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Electronic Structure of Defects in the Thomas–Fermi–von Weizsäcker Model of Crystals

by

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Declarations

The majority of the work presented in this thesis was done in collaboration with my supervisor Christoph Ortner.

- Results in Chapters 2,3,4,5 regarding the existence, uniqueness and locality of the TFW Coulomb ground states and the construction of site energies can be found in Nazar, Ortner (Arxiv preprint, 2015).

- Similarly, the analogous results for TFW Yukawa systems, also presented in Chapters 2,3,4,5, can be found in Nazar (Arxiv preprint, 2016).

- In addition, the content presented in Chapter 6 is mostly a simplified version of joint work with Christoph Ortner and Huajie Chen [2], which is in preparation.

I declare that to the best of my knowledge, the material contained in this thesis is original and my own work except where otherwise stated. This thesis has not been submitted for a degree at any other university.

Abstract

In this thesis, we establish a locality property for solutions to the Thomas–Fermi–von Weizsäcker (TFW) equations. This is a system of coupled PDEs that models the ground state electron density corresponding to a given nuclear arrangement. The locality property is a pointwise stability estimate for the TFW equations, that demonstrates the exponential response of the electron density to a perturbation of the nuclei. We show that this result holds for the TFW when using either the Coulomb or the Yukawa potential to treat the interaction of charged particles.

We then use the locality result to prove several consequences for the TFW ground state, which includes generalising results from [14] regarding the neutrality of infinite systems and also showing the uniform convergence of ground states when passing to the limit from the Yukawa to the Coulomb model.

Our main application is the construction of site energies from the TFW energy. The locality result implies that the response of each site energy decays exponentially with respect to a perturbation of the nuclear arrangement. Using these site energies, we then formulate the lattice relaxation problem, that was initially formulated in [23], to consider the response of a perfect crystal lattice to the introduction of a point defect. The site energies allow us to formulate a variational problem over a space of deformations of the lattice, show this problem is well-posed and finally establish the decay properties of minimisers.

Chapter 1

Introduction

Crystalline solids are commonly found in both nature and everyday life. Some familiar examples include table salt (sodium chloride) and quartz crystals, which are used in timekeeping devices. The physical structure of crystals are characterised by periodic arrangement of atoms or molecules. However, imperfections, or defects exist in most crystals, which can affect the physical properties of the material. Line defects called dislocations affect the plastic deformation of the material [32], while large concentrations of point defects can alter the conductivity of the crystal. The latter property is used in the manufacture of semiconductor devices in a process known as doping [31].

Our interest is in studying the effects of introducing defects[1] into crystals at the atomic scale, where it becomes necessary to consider atoms in terms of their constituent nuclei and electrons. At this scale, quantum effects become significant, which includes the charge interaction of nuclei and electrons via the long-ranged Coulomb potential. Our aim is to find the equilibrium configuration of the defective crystal, by investigating an associated energy minimisation problem.

A significant challenge stems from dealing with the high-dimensional nature of such problems, when formulated at the quantum level. For this reason, it becomes necessary to reduce the complexity of the problem, such as applying the Born–Oppenheimer approximation [11, 40]. It is a well-established technique that allows for the separation the electronic and nuclear behaviour

[1] A detailed introduction to the mathematical modelling of point defect in crystals can be found in [13].

under the assumption that the electrons lie in equilibrium with respect to the nuclear configuration, due to the large relative mass of a nucleus compared to an electron. Hence, one can first fix a trial nuclear arrangement, solve for the corresponding electron ground state and then optimise over the nuclear configurations to find an approximate equilibrium and total energy for the full system. In the literature, this final step is called geometry optimisation [10, 13].

To obtain the electron ground state for a fixed nuclear configuration, one could in-principle solve the full time-independent Schrödinger equation for the electron wavefunction. However, as this quickly becomes intractable as the number of particles in the system grows, Density Functional Theory (DFT) is commonly used instead. The key idea of DFT is that the electron minimisation problem can be formulated solely in terms of the electron density, as opposed to the full wavefunction. This theory was first introduced by Hohenberg and Kohn [30] and developed further by Lieb [48] and Levy [44].

In DFT, one finds the electron ground state by minimising an energy functional over a space of trial electron densities. Its main drawback is that an exact form for the functional is unknown. Instead, for both numerical and theoretical purposes, there are many approximate mean-field energy functionals used in the DFT setting, such as the Thomas–Fermi–von Weizsäcker (TFW), Hartree–Fock (HF) and Kohn–Sham (KS) models [22]. The TFW model describes the electron behaviour in terms of a density function defined on $\mathbb{R}^3$, whereas both HF and KS are defined using density matrices and incorporate the antisymmetry constraint imposed by Pauli's Exclusion Principle, since electrons are classified as fermions. As the TFW model is constructed using only the electron density, it is called an orbital-free model. Due to this, it also fails to take antisymmetry into account. For these reasons, the TFW model is simpler, but less accurate than either the HF or KS models.

Consequently the TFW model is less commonly used in electronic structure calculations, however many aspects of its mathematical analysis are still relevant for more advanced models.

The TFW model belongs to a family of orbital-free models that predate DFT. The original model, the Thomas–Fermi (TF) model, introduced independently by Thomas [64] and Fermi [25] in 1927, describes the electrons as a homogeneous gas. It was later studied in a mathematical setting by Lieb and Simon [46]. A significant shortcoming of TF theory is that binding of atoms to form molecules does not occur in this model, a result known in the literature as Teller's No Binding Theorem [63].

In 1935, von Weizsäcker introduced a inhomogeneity correction term [65] to the kinetic energy, which allows binding to occur in the TFW model [6]. Given a sufficiently regular nuclear charge density $m : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$, the TFW energy is given by

$$E^{\mathrm{TFW}}(\sqrt{\rho}, m) = C_{\mathrm{W}} \int_{\mathbb{R}^3} |\nabla \sqrt{\rho}|^2 + C_{\mathrm{TF}} \int_{\mathbb{R}^3} \rho^{5/3} \\ + \frac{1}{2} \int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{(m-\rho)(x)(m-\rho)(y)}{|x-y|} \, \mathrm{d}x \, \mathrm{d}y, \qquad (1.1)$$

where $\rho : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$ corresponds to the electron density. Several values have been proposed for the nonnegative constant C_{W} [22], while the TF model corresponds to choosing $C_{\mathrm{W}} = 0$. This form of the TFW energy is strictly convex in ρ.

As neither of the TF and TFW models consider antisymmetry of electrons, to compensate for this, in 1928 Dirac proposed adding an exchange term of the form $-C_D \int_{\mathbb{R}^3} \rho^{4/3}$ to (1.1), which gives rise to the Thomas–Fermi–Dirac–von Weizsäcker (TFDW) model [20]. Unfortunately, the introduction of the exchange term removes the strict convexity of the energy functional. As a result, the potential lack of uniqueness of minimisers becomes a significant technical issue [49, 43]. Moreover, a result on the non-existence of minimisers has also been shown for this model [50].

By comparison, in the TFW setting, the uniqueness of minimisers for finite systems is an immediate consequence of the strict convexity of the functional. As the TFW energy per unit volume remains bounded with system size, one can not identify the ground state for infinite systems as the minimiser of a variational problem. Instead, ground states for infinite systems are constructed using a thermodynamic limit argument [16]. In particular, this is used to find the ground state corresponding to a perfect crystal lattice.

The supercell method is one such procedure to compute the electronic structure of a perfect crystal with a local defect. This approach has the advantage of utilising the periodicity of the reference crystal, hence Bloch–Floquet theory is applicable [58]. By constructing a supercell, that is a large domain with periodic boundary conditions chosen to match the periodicity of the perfect lattice, one can find the electronic structure of a crystal with a local defect by sending the size of the supercell to infinity. This procedure has been applied to study defects in both the TFW and the restricted Hartree–Fock[2] (rHF) models [14, 15]. It has also been shown that the local defects are charge-neutral in the TFW setting, whereas local defects may introduce a charge in the rHF model.

Alternatively, for infinite nuclear configurations that do not possess any underlying symmetry, a general approach to constructing the corresponding ground state is possible in the TFW setting. Consider a suitable nuclear distribution $m : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$ corresponding to an infinite collection of nuclei and define for each $R > 0$ the truncation $m_R = m \cdot \chi_{B_R}$. Then, one can find a unique minimiser u_R to the corresponding variational problem[3]

$$I^{\mathrm{TFW}}(m_R) = \inf \left\{ E^{\mathrm{TFW}}(v, m_R) \,\middle|\, v \in H^1(\mathbb{R}^3), v \geq 0, \int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m_R \right\}. \tag{1.2}$$

Passing to the limit as $R \to \infty$ yields the infinite ground state $u = \lim_{R\to\infty} u_R$. This technique holds for a broad range of nuclear distributions for the TFW model. In comparison to the supercell method, the uniform estimates required to pass to the limit in the more general setting are significantly more challenging to show for more advanced models. This general approach is considered in depth in [16].

As a significant challenge in finding electron ground states comes from dealing with the interaction of charged particles via the long-ranged Coulomb potential $\frac{1}{|x|}$, the short-ranged Yukawa potential $Y_a(x) = \frac{e^{-a|x|}}{|x|}$, with parameter

[2]The rHF model is defined by removing the exchange term from the HF functional, which ensures that the resulting functional is strictly convex. While existence results for finite systems have been shown in the full HF setting [49], the rHF model avoids the technical issue of nonconvexity of the energy functional and allows one to pass to the thermodynamic limit to study infinite systems.

[3]The constraint in (1.2) ensures that the total system is charge neutral and is a convenient assumption. Existence and uniqueness has also been shown for finite non-neutral systems and allows for positively charged ions to exists in the TFW setting [6, 62].

$a > 0$, is a commonly used approximation. The parameter a is interpreted in the physical setting as the screening length [38]. When considering Y_a as a Green's function, it can also be viewed as a regularisation of the Poisson equation to give the screened Poisson equation [60]. The TFW model with Yukawa potential is also considered in detail in [16], and the convergence of the energy per unit volume is shown for periodic systems, when passing from the Yukawa to the Coulomb potential by sending $a \to 0$.[4]

1.1 Main results of the thesis

Broadly speaking, in the mathematical literature, considerable progress has been made on studying electrons ground states corresponding to local defects in crystals, whereas much less is understood about the related geometry optimisation problem [26], which we refer to as the lattice relaxation problem.

The primary goal of this work is to explore the lattice relaxation problem, which investigates the rearrangement caused by the introduction of a local defect into a perfect crystal, using the TFW model. We consider the static zero temperature problem, so we search for equilibrium configurations once relaxation has completed. The challenge of this problem is that lattice relaxation is a mechanical process involving the rearrangement of nuclei.

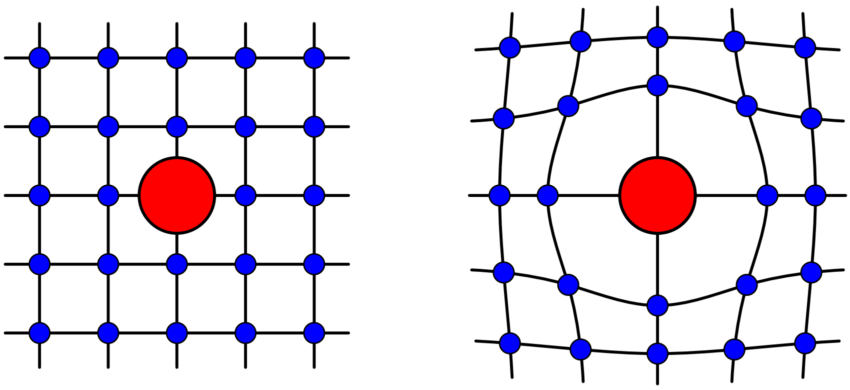


Figure 1.1: A diagram showing a lattice containing a point defect before and after relaxation.

[4]The rHF model with Yukawa interaction has also been studied in [42], which establishes the response of the rHF electron density and mean-field potential to a local defect in an otherwise perfect crystal.

We remark that geometry optimisation in the TFW model has been studied in [10], which introduces a variational problem that minimises the TFW energy over a class of nuclear arrangements. However, the variational problem in [10] exclusively considered periodic systems, whereas in the lattice relaxation problem, the introduction of a local defect breaks the periodicity of the crystal.

In recent work, local defects in crystals have been studied for electronic structure models using the supercell method [13]. In these problems, once the defect is introduced, the perturbed nuclear arrangement is fixed in the analysis.

To study the lattice relaxation problem, it is necessary to consider large deformations that affect the entire lattice. This requires treating nuclear configurations that differ everywhere from the periodic arrangement. Consequently, the supercell approach is no longer applicable. Instead, we apply the more general thermodynamic limit argument (1.2), presented in [16] to define the electron density corresponding to a nuclear configuration, for a general condensed phase.

While the lattice relaxation problem is open for electronic structure models, it has been studied using energies constructed from classical interatomic potentials [23]. Moreover, both point defects and straight line dislocations have been treated in this setting. For our purposes, the significant contributions of [23] are to formulate the lattice relaxation problem as a variational problem, show it is well-posed and establish decay results for minimising lattice arrangements.

A key issue is that the form of the TFW energy differs considerably from the energy used in [23], which are defined as the sum of site energies that depend only on nearby particles: given a countable collection of nuclei $Y = (Y_k)_{k \in \mathbb{N}} \subset \mathbb{R}^3$, let

$$E_j^{\mathrm{MM}}(Y) = \sum_{|Y_i - Y_j| \leq r_{\mathrm{cut}}} V\big(|Y_i - Y_j|\big), \tag{1.3}$$

where $V : \mathbb{R} \to \mathbb{R}$ is a smooth interatomic potential and $r_{\mathrm{cut}} > 0$ imposes a finite radius of interaction. In comparison, recall that the TFW energy (1.1) is given by an integral over $\mathbb{R}^3$ that depends on the entire nuclear configuration

$Y = (Y_k)_{k\in\mathbb{N}}$. Consequently, in order to apply the ideas from [23], we must first show that the TFW energy can be decomposed into energy contributions that have a *local* dependence on the surrounding nuclei.

As the TFW energy (1.1) depends on both the nuclear configuration and the corresponding electron density, it is necessary to understand how the electron density responds to a perturbation of the nuclear arrangement. For example, given a nuclear arrangement with a well-behaved electron ground state, consider the effect of applying a small perturbation to one nucleus in the arrangement, while keeping the other nuclei fixed. Due to the long-ranged Coulomb interaction, it is plausible that the resulting response of the electron ground state may be long-ranged. We show the following result, which justifies that this is not the case and rather the response of the ground state decays exponentially with distance from the nuclear perturbation.

In Chapter 3, we show a general locality estimate for the TFW model, which can be thought of as a pointwise stability estimate for the TFW equations (1.4). This comes from adapting and generalising the uniqueness result proof from [16].

Theorem. *For $i = 1, 2$, let $m_i \in L^\infty(\mathbb{R}^3)$ represent nuclear charge distributions satisfying*

$$m_i \geq 0 \qquad \textit{and} \qquad \lim_{R\to\infty} \frac{1}{R} \inf_{x\in\mathbb{R}^3} \int_{B_R(x)} m_i(z)\, \mathrm{d}z = +\infty.$$

Let the corresponding ground state electron densities and electrostatic potentials, denoted by $u_i, \phi_i : \mathbb{R}^3 \to \mathbb{R}$, satisfy the TFW equations,

$$\begin{aligned} -\Delta u_i + \frac{5}{3} u_i^{7/3} - \phi_i u_i &= 0, \\ -\Delta \phi_i &= 4\pi(m_i - u_i^2), \end{aligned}$$

Then there exists $C, \gamma > 0$ such that for all $y \in \mathbb{R}^3$

$$|(u_1 - u_2)(y)| + |(\phi_1 - \phi_2)(y)| \leq C \left(\int_{\mathbb{R}^3} |(m_1 - m_2)(x)|^2 e^{-2\gamma|x-y|}\, \mathrm{d}x \right)^{1/2}. \tag{1.5}$$

The locality estimate (1.5) can be interpreted as a screening result for the TFW model, which explains the exponential decay of the electron response despite the long-ranged Coulomb interaction. This is discussed in detail in Chapter 4.

Additionally, locality properties of electronic structure models are a key premise in certain state of the art numerical algorithms. A well-established example is near-sightedness, a locality property of the density matrix which gives rise to linear scaling algorithms for KS type models [33, 57, 29, 7]. A stronger notion is the locality of the mechanical response, which is a fundamental premise underpinning the construction of interatomic potentials and of multi-scale algorithms such as hybrid QM/MM schemes [19] (here, it is called strong locality). The estimate (1.5) falls under the latter category, which is less well studied as the only result in this direction is the locality of non-selfconsistent tight binding models [17].

Using (1.5), in Chapter 5 we decompose the TFW energy for an infinite system into individual site energies for each nucleus. The key property is that the response of each site energy to a nuclear perturbation decays exponentially with their distance, in the following sense.

Given a countable collection of nuclei $Y = (Y_k)_{k\in\mathbb{N}} \subset \mathbb{R}^3$ we construct an energy density $\mathcal{E}(Y; x)$, as follows. Using Y we define a nuclear charge density $m = m_Y$, then find the corresponding ground state (u, ϕ) by solving the TFW equations. One possible choice of energy density is given by

$$\mathcal{E}(Y; \cdot) = |\nabla u|^2 + u^{10/3} + \frac{1}{2}\phi\left(m - u^2\right).$$

This allows us to define the TFW energy $\int_\Omega \mathcal{E}(Y; x)\,\mathrm{d}x$ of an arbitrary volume $\Omega \subset \mathbb{R}^3$ in a meaningful way and motivates us to define site energies

$$E_j(Y) := \int_{\mathbb{R}^3} \varphi_j(x)\mathcal{E}(Y; x)\,\mathrm{d}x, \tag{1.6}$$

where $(\varphi_j)_{j\in\mathbb{N}}$ is a smooth partition of unity of $\mathbb{R}^3$, which can be constructed in such a way that E_j are permutation and isometry invariant and most crucially,

E_j are *local* in the sense that

$$\left| \frac{\partial E_j(Y)}{\partial Y_k} \right| \leq C e^{-\gamma |Y_j - Y_k|}, \tag{1.7}$$

for some $C, \gamma > 0$. We also show similar estimates for higher derivatives of the site energies, which requires showing the existence, uniqueness and locality of the higher variations of the TFW equations. Solutions of the linearised TFW equations have been shown to exist and be unique in [8] and we extend this to all variations of the TFW equations.

The site energy construction (1.6) allows us to treat the TFW model as a classical interatomic potential (for example the Lennard–Jones interatomic potential [34]) and in particular enables us to extend the analysis of the lattice relaxation problem [23] to the TFW model. In [23], it is assumed that site energy potentials (1.3) have finite interaction range, i.e. the site energy potential depends only on particles within a fixed radius. This does not hold for the TFW model, as (1.7) demonstrates that the site energy $E_j(Y)$ depends on the entire nuclear configuration $Y = (Y_k)_{k \in \mathbb{N}}$. Therefore careful analysis is required to show that the variational framework detailed in [23] supports the TFW model.

To this end, we define a variational problem for nuclear deformations using the TFW energy. In Chapter 6, we define an admissible space $\dot{\mathscr{W}}^{1,2}(\Lambda)$ of nuclear perturbations of the defective lattice, where $\dot{\mathscr{W}}^{1,2}(\Lambda)$ is a canonical discrete variant of the homogeneous Sobolev space $\dot{H}^1(\mathbb{R}^3)$. Then using the TFW site energies, we assign an energy $\mathscr{E}(U)$ to each $U \in \dot{\mathscr{W}}^{1,2}(\Lambda)$ using (1.6). Let Y_0 represent the nuclear arrangement of the defective lattice before relaxation, then define

$$\mathscr{E}(U) = \sum_{j=1}^{\infty} \big(E_j(Y_0 + U) - E_j(Y_0) \big). \tag{1.8}$$

This associates an energy difference to each $U \in \dot{\mathscr{W}}^{1,2}(\Lambda)$ by comparing the energy at $Y_0 + U$ to the reference configuration Y_0. Using estimates similar to (1.7), we show that the energy difference (1.8) is well-defined hence we are able to identify the thermodynamic limit variational problem:

$$\text{Find } \bar{U} \in \arg\min \left\{ \mathscr{E}(U) \,\middle|\, U \in \dot{\mathscr{W}}^{1,2}(\Lambda) \right\}. \tag{1.9}$$

We then show that any minimiser possesses the decay property

$$\left|\bar{U}(\ell)\right| \leq C\big(1 + |\ell|\big)^{-2}. \tag{1.10}$$

To our knowledge, this is the first result incorporating both electronic structure theory and lattice mechanics in a mathematical setting. As the tight-binding and rHF with Yukawa interaction models have also been shown to satisfy locality properties [17, 42], once estimates of the form (1.7) have been established, the framework presented in Chapter 6 for the lattice relaxation problem can be immediately applied to these models, though we do not pursue this here.

We now briefly mention further applications of the locality estimates (1.5) which are discussed in Chapter 4. A significant application of (1.5) is to compare TFW ground states defined by the Coulomb and Yukawa potential. For a fixed nuclear distribution m, suppose (u, ϕ) and (u_a, ϕ_a) are the corresponding Coulomb and Yukawa ground states, for $a > 0$. Then, we show the uniform convergence of ground states, in terms of the Yukawa parameter a,

$$\|u_a - u\|_{L^\infty(\mathbb{R}^3)} + \|\phi_a - \phi\|_{L^\infty(\mathbb{R}^3)} \leq Ca^2. \tag{1.11}$$

To the best of our knowledge, this is the first result to show pointwise convergence of ground states from Yukawa to Coulomb for any electronic structure model. The closest existing result to (4.13) we have found in the literature is [16, Proposition 2.30], which shows $u_a \to u$ strongly in $H^1_{\text{loc}}(\mathbb{R}^3)$ as $a \to 0$, for periodic and neutral TFW systems, but does not estimate the rate.

An additional application extends the neutrality estimate presented in [14] to non-periodic nuclear configurations. Moreover, the decay rate of minimising displacements (1.10) is sufficient to show that after the defective system has reached equilibrium after undergoing relaxation, the system remains charge-neutral.

Also, in Section 4.1, we establish the exponential convergence of ground states over compact sets via the thermodynamic limit procedure, which generalises and strengthens results shown for thin films in the TFW model [9] to general nuclear configurations.

1.2 Outline of thesis

Chapter 2 - In this chapter, we provide an overview of the TFW model, with both Coulomb and Yukawa interaction. We give an overview of the existence and uniqueness of ground states of the associated system of Euler–Lagrange equations, which we refer to as the TFW equations. While existence and uniqueness of the TFW equations for infinite nuclear configurations has been covered in detail in [16], we revisit the proofs in order to establish uniform regularity estimates for the ground states, which will be used readily throughout this work.

Chapter 3 - Once uniform regularity estimates have been established, we turn our attention to establishing locality estimates such as (1.5), for both the Coulomb and Yukawa systems. These are the main technical results of the thesis. As an application, we show how the electron response inherits the decay properties of the nuclear perturbations.

Chapter 4 - Here we collect the further applications of (1.5), discussed in the previous section.

In the subsequent chapters, we work entirely in the Coulomb setting, though we remark that the entire analysis holds verbatim in the Yukawa setting.

Chapter 5 - The next chapter is devoted to constructing the site energies and showing their exponential decay with respect to nuclear perturbations. This involves solving higher variations of the TFW equations, so we also show existence, uniqueness and locality results for all variations.

Chapter 6 - In the final chapter, we introduce the lattice relaxation problem for point defects in the TFW model. We apply the site energy results from Chapter 5 to show the minimisation problem (1.9) is well-defined and establish the decay of minimisers.

Chapter 2

The Thomas–Fermi–von Weizsäcker Model

2.1 Background

Throughout the thesis, C will be used to denote a positive constant, whose value may increase from line to line. The dependence of the constant C on other parameters will be made clear in the statement of each individual result.

For $p \in [1, \infty]$ define the function spaces

$$L^p_{\mathrm{loc}}(\mathbb{R}^3) := \{\, f : \mathbb{R}^3 \to \mathbb{R} \,|\, \forall\, K \subset \mathbb{R}^3 \text{ compact}, f \in L^p(K) \,\} \quad \text{and}$$
$$L^p_{\mathrm{unif}}(\mathbb{R}^3) := \{\, f \in L^p_{\mathrm{loc}}(\mathbb{R}^3) \,|\, \sup_{x \in \mathbb{R}^3} \|f\|_{L^p(B_1(x))} < \infty \,\}.$$

For $k \in \mathbb{N}$, $H^k_{\mathrm{loc}}(\mathbb{R}^3), H^k_{\mathrm{unif}}(\mathbb{R}^3)$ are defined analogously. For a multi-index $\alpha = (\alpha_1, \alpha_2, \alpha_3)$, define the partial derivative $\partial^\alpha = \partial_1^{\alpha_1} \partial_2^{\alpha_2} \partial_3^{\alpha_3}$. Throughout this paper, α, β denote three-dimensional multi-indices.

The Coulomb interaction, for $f, g \in L^{6/5}(\mathbb{R}^3)$, is given by

$$D_0(f, g) = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{f(x) g(y)}{|x - y|} \,\mathrm{d}x \,\mathrm{d}y = \int_{\mathbb{R}^3} \left(f * \tfrac{1}{|\cdot|} \right)(y) g(y) \,\mathrm{d}y.$$

and is finite due to the Hardy–Littlewood–Sobolev estimate [4]

$$|D_0(f, g)| \leq \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|f(x)||g(y)|}{|x - y|} \,\mathrm{d}x \,\mathrm{d}y \leq C \|f\|_{L^{6/5}(\mathbb{R}^3)} \|g\|_{L^{6/5}(\mathbb{R}^3)}.$$

The Yukawa interaction is a short-range approximation to the Coulomb interaction, with the Yukawa potential $Y_a(x) = \frac{e^{-a|x|}}{|x|}$, for $a > 0$, replacing the Coulomb potential $\frac{1}{|x|}$. The parameter $a > 0$ controls the range of the interaction, in particular one formally recovers the long-ranged Coulomb interaction as $a \to 0$. The Yukawa interaction, for $a > 0$ and $f, g \in L^2(\mathbb{R}^3)$, is given by

$$D_a(f,g) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{f(x)e^{-a|x-y|}g(y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y = \int_{\mathbb{R}^3} \left(f * Y_a\right)(y)g(y)\,\mathrm{d}y,$$

which is finite as the Cauchy-Schwarz and Young inequalities for convolutions imply

$$|D_a(f,g)| \leq \|Y_a\|_{L^1(\mathbb{R}^3)}\|f\|_{L^2(\mathbb{R}^3)}\|g\|_{L^2(\mathbb{R}^3)} \leq Ca^{-2}\|f\|_{L^2(\mathbb{R}^3)}\|g\|_{L^2(\mathbb{R}^3)}.$$

Let $m \in L^{6/5}(\mathbb{R}^3), m \geq 0$ denote the charge density of a finite nuclear cluster, then the corresponding TFW Coulomb energy functional is defined, for $v \in H^1(\mathbb{R}^3)$, by

$$E^{\mathrm{TFW}}(v,m) = C_{\mathrm{W}}\int_{\mathbb{R}^3}|\nabla v|^2 + C_{\mathrm{TF}}\int_{\mathbb{R}^3} v^{10/3} + \frac{1}{2}D_0(m-v^2, m-v^2). \tag{2.1}$$

The function v corresponds to the positive square root of the electron density. The first two terms of $E^{\mathrm{TFW}}(v,m)$ model the kinetic energy of the electrons while the third term models the Coulomb energy. We remark that this definition of the Coulomb energy is only valid for *smeared nuclei*[1]. We can rescale the energy to ensure $C_{\mathrm{W}} = C_{\mathrm{TF}} = 1$, while leaving the constant appearing in front of the Coulomb interaction term unchanged.

Also, let $a > 0$ and $m \in L^2(\mathbb{R}^3), m \geq 0$, denote the charge density of a finite nuclear cluster, then the corresponding TFW Yukawa energy functional

[1] In electronic structure theory, nuclei are modelled either by a smeared or point description. Consider a collection of M nuclei with positive charges $(z_k)_{1\leq k\leq M}$, located at $(R_k)_{1\leq k\leq M} \subset \mathbb{R}^3$. In the smeared nuclei setting, the nuclear charge distributions is modelled by $\sum_{k=1}^{M} z_k\delta(x - R_k)$, where δ is the Dirac measure at 0. In comparison, the smeared nuclear setting replaces δ with $\eta \in C_{\mathrm{c}}^{\infty}(\mathbb{R}^3)$ satisfying $\eta \geq 0$, radial, centred at 0 and $\int_{\mathbb{R}^3}\eta = 1$. This removes the singularity at each nucleus, which simplifies the analysis of the TFW equations [16].

is defined, for $v \in H^1(\mathbb{R}^3)$, by

$$E_a^{\mathrm{TFW}}(v,m) = C_{\mathrm{W}} \int_{\mathbb{R}^3} |\nabla v|^2 + C_{\mathrm{TF}} \int_{\mathbb{R}^3} v^{10/3} + \frac{1}{2} D_a(m - v^2, m - v^2),$$

which replaces the Coulomb interaction term in (2.1) with a Yukawa interaction term.

To construct the electronic ground state for an infinite arrangement of nuclei (e.g., crystals), it is necessary to restrict admissible nuclear charge densities to $m \in L^1_{\mathrm{unif}}(\mathbb{R}^3), m \geq 0$, satisfying

$$\sup_{x \in \mathbb{R}^3} \int_{B_1(x)} m(z) \, \mathrm{d}z < \infty, \tag{H1}$$

$$\lim_{R \to \infty} \inf_{x \in \mathbb{R}^3} \frac{1}{R} \int_{B_R(x)} m(z) \, \mathrm{d}z = \infty. \tag{H2}$$

The property (H1) guarantees that no clustering of infinitely many nuclei occurs at any point in space whereas (H2) ensures that there are no large regions that are devoid of nuclei.

Now consider the system: $u \geq 0$ and

$$-\Delta u + \frac{5}{3} u^{7/3} - \phi u = 0, \tag{2.2a}$$

$$-\Delta \phi = 4\pi(m - u^2). \tag{2.2b}$$

We refer to (u, ϕ) as a *ground state* corresponding to m. The existence and uniqueness of ground states is guaranteed by [16, Theorem 6.10]. Similarly, for $a > 0$, consider the alternative system: $u_a \geq 0$ and

$$-\Delta u_a + \frac{5}{3} u_a^{7/3} - \phi_a u_a = 0, \tag{2.3a}$$

$$-\Delta \phi_a + a^2 \phi_a = 4\pi(m - u_a^2). \tag{2.3b}$$

We refer to (u_a, ϕ_a) as a *Yukawa ground state* corresponding to m. As remarked in [16, Chapter 6], it also follows that for sufficiently small $a > 0$, the existence and uniqueness of the Yukawa ground state (u_a, ϕ_a) is also guaranteed.

The equation (2.2b) arises from the Coulomb interaction, as $\frac{1}{4\pi|\cdot|}$ is the Green's function for the Laplacian on $\mathbb{R}^3$, while (2.3b) is obtained for the

Yukawa problem, as $\frac{1}{4\pi}Y_a$ is the Green's function for $-\Delta + a^2$ on $\mathbb{R}^3$, $a > 0$.

Definition 1. *For any nuclear configuration m satisfying* (H1)–(H2)*, the Coulomb ground state corresponding to m refers to the unique solution (u, ϕ) to* (2.2) *satisfying $u \geq 0$. For $a > 0$, the Yukawa ground state corresponding to m refers to the unique solution (u_a, ϕ_a) solving* (2.3) *and satisfying $u_a \geq 0$.* $\square$

2.2 Main results

The aim of this chapter is to review the existence and uniqueness of the TFW equations and to prove uniform regularity estimates for the solutions. These results rely on uniform variants of (H1)–(H2), which we describe using the following spaces. Given $M, \omega_0, \omega_1 > 0$, let $\omega = (\omega_0, \omega_1)$ and define the class of nuclear configurations

$$\mathcal{M}_{L^2}(M,\omega) = \left\{ m \in L^2_{\mathrm{unif}}(\mathbb{R}^3) \;\middle|\; \|m\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq M, \right. \\ \left. \forall\, R > 0 \;\inf_{x\in\mathbb{R}^3} \int_{B_R(x)} m(z)\,\mathrm{d}z \geq \omega_0 R^3 - \omega_1 \right\}. \tag{2.4}$$

Clearly, as $L^2_{\mathrm{unif}}(\mathbb{R}^3) \subset L^1_{\mathrm{unif}}(\mathbb{R}^3)$, any $m \in \mathcal{M}_{L^2}(M,\omega)$ satisfies (H1). Moreover, in Lemma 2.8, we show an equivalence between the second condition of (2.4) and (H2). As each nuclear distribution $m \in \mathcal{M}_{L^2}(M,\omega)$ satisfies (H1)–(H2) [16, Theorem 6.10] guarantees the existence of corresponding Coulomb (u, ϕ) and Yukawa (u_a, ϕ_a) ground states, for sufficiently small a.

We also introduce the following spaces, as assuming higher regularity of the nuclear distributions implies higher regularity of the ground state. For $k \in \mathbb{N}_0$, define

$$\mathcal{M}_{H^k}(M,\omega) = \left\{ m \in H^k_{\mathrm{unif}}(\mathbb{R}^3) \;\middle|\; \|m\|_{H^k_{\mathrm{unif}}(\mathbb{R}^3)} \leq M, \right. \\ \left. \forall\, R > 0 \;\inf_{x\in\mathbb{R}^3} \int_{B_R(x)} m(z)\,\mathrm{d}z \geq \omega_0 R^3 - \omega_1 \right\}.$$

Remark 1. We have chosen our spaces $\mathcal{M}_{L^2}, \mathcal{M}_{H^k}$ to ensure that $m \in L^2_{\mathrm{unif}}(\mathbb{R}^3)$, which allows us to apply L^2-regularity theory for elliptic partial differential equations. However, the proof of [16, Theorem 6.10] holds for $m \in L^1_{\mathrm{unif}}(\mathbb{R}^3)$ satisfying (H2). Consequently, we believe that the analysis presented in this chapter will continue to hold if one instead m belonging to

$$\mathcal{M}_{L^1}(M,\omega) = \left\{ m \in L^1_{\mathrm{unif}}(\mathbb{R}^3) \;\middle|\; \|m\|_{L^1_{\mathrm{unif}}(\mathbb{R}^3)} \leq M, \right.$$
$$\left. \forall\, R > 0 \; \inf_{x \in \mathbb{R}^3} \int_{B_R(x)} m(z)\, \mathrm{d}z \geq \omega_0 R^3 - \omega_1 \right\}.$$

We give the general existence and uniqueness results for both the Coulomb and Yukawa settings.

2.2.1 Coulomb existence and uniqueness

Proposition 2.1. *For any nuclear distribution $m : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$, satisfying*

$$\|m\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq M,$$

there exists (u, ϕ) solving (2.2) and satisfying $u \geq 0$ and

$$\|u\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(1 + M^{15/4}), \tag{2.5}$$
$$\|\phi\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(1 + M^{3/2}). \tag{2.6}$$

We now state the uniqueness result for Coulomb ground states. This relies on showing lower bounds for the electron density, so we also generalise the argument presented in [16, Lemma 5.3, Theorem 6.10] to ensure these estimates are uniform for ground states corresponding to $m \in \mathcal{M}_{L^2}(M, \omega)$.

Proposition 2.2. *There exists $c_{M,\omega} > 0$ such that for all $m \in \mathcal{M}_{L^2}(M, \omega)$ the corresponding ground state $(u, \phi) \in H^4_{\mathrm{unif}}(\mathbb{R}^3) \times H^2_{\mathrm{unif}}(\mathbb{R}^3)$ is unique and the electron density u satisfies*

$$\inf_{x \in \mathbb{R}^3} u(x) \geq c_{M,\omega} > 0.$$

Assuming higher regularity of the nuclear configuration yields additional regularity estimates for the corresponding ground state. The following result makes use of the uniform lower bound established in Proposition 2.2.

Corollary 2.3. *Suppose $k \in \mathbb{N}_0$ and $m \in \mathcal{M}_{H^k}(M,\omega)$, then the corresponding solution (u,ϕ) to (2.2) satisfies*

$$\|u\|_{H^{k+4}_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi\|_{H^{k+2}_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(k,M,\omega).$$

Remark 2. The existence and uniqueness for Coulomb systems has been shown in detail in [16, Theorem 6.10], whereas the uniform regularity estimates presented in Propositions 2.1, 2.2 and Corollary 2.3 are new results. The uniformity of these upper and lower bounds are significant as they directly control the rate of exponential decay in the locality results we will establish in Chapter 3. □

2.2.2 Yukawa existence and uniqueness

In the Coulomb setting, Proposition 2.1 gives the existence and regularity estimates for any $m \in L^2_{\mathrm{unif}}(\mathbb{R}^3)$. In comparison, to show existence of solutions in the Yukawa setting, it is necessary to differentiate between nuclear arrangements $m \in L^2_{\mathrm{unif}}(\mathbb{R}^3), m \not\equiv 0$ and those satisfying the stronger condition $m \in \mathcal{M}_{L^2}(M,\omega)$. When $m \in \mathcal{M}_{L^2}(M,\omega)$, we can show the Yukawa ground state (u_a,ϕ_a) exists for all $a > 0$, whereas in the former case, we only show the existence of a ground state for sufficiently small $a > 0$.

Proposition 2.4. *For any nuclear distribution $m : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$, satisfying*

$$\|m\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq M,$$

there exists $a_0 = a_0(m) > 0$ such that for all $0 < a \leq a_0$, there exists (u_a,ϕ_a) solving (2.3), satisfying $u_a \geq 0$ and

$$\|u_a\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_a\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M).$$

If $\int_{B_{R_0}(x)} m \geq c_0 > 0$ for some $x \in \mathbb{R}^3$ and $R_0, c_0 > 0$, then $a_0 = a_0(R_0,c_0) > 0$.

Proposition 2.4 will be used in the proof of Proposition 4.2, which compares the Yukawa ground state with its finite approximation.

Proposition 2.5. *Let $a_0 > 0$ and $m \in \mathcal{M}_{L^2}(M, \omega)$, then for any $0 < a \leq a_0$ there exists (u_a, ϕ_a) solving (2.3), satisfying $u_a \geq 0$ and*

$$\|u_a\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_a\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(a_0, M), \tag{2.7}$$

where the constant $C(a_0, M)$ is increasing in both a_0 and M.

We now state the uniqueness result for Yukawa ground states. The only difference between uniqueness in the Coulomb and Yukawa models is that the uniform lower bound for Yukawa ground state electron density depends on the value of the screening parameter, $a > 0$.

A formal justification gives that as a grows, the term $a^2\phi_a$ dominates the left-hand side of (2.3b), so one may expect that $\phi_a \to 0$ as $a \to \infty$. In this case, sending $a \to \infty$ in (2.3a) gives $-\Delta u + \frac{5}{3}u^{7/3} = 0$, which has the trivial solution $u \equiv 0$.

Proposition 2.6. *Let $a_0 > 0$ and $m \in \mathcal{M}_{L^2}(M, \omega)$, then for all $0 < a \leq a_0$ the corresponding Yukawa ground state $(u_a, \phi_a) \in H^4_{\mathrm{unif}}(\mathbb{R}^3) \times H^2_{\mathrm{unif}}(\mathbb{R}^3)$ is unique and there exists $c_{a_0,M,\omega} > 0$ such that the electron density u_a satisfies*

$$\inf_{x \in \mathbb{R}^3} u_a(x) \geq c_{a_0,M,\omega} > 0.$$

When the nuclear configuration possesses additional regularity, we also obtain additional regularity estimates for the corresponding Yukawa ground state.

Corollary 2.7. *Let $a_0 > 0$, $k \in \mathbb{N}_0$ and $m \in \mathcal{M}_{H^k}(M, \omega)$, then for all $0 < a \leq a_0$ the corresponding Yukawa ground state (u_a, ϕ_a) satisfies*

$$\|u_a\|_{H^{k+4}_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_a\|_{H^{k+2}_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(a_0, k, M, \omega).$$

Remark 3. The existence and uniqueness of the TFW Yukawa ground state is discussed in detail for periodic systems in [16, Chapters 2,4] while the discussion in [16, Chapter 6] asserts that the main existence and uniqueness result for general nuclear configurations [16, Theorem 6.10] follows verbatim for Yukawa systems. However, the proof of this result makes use of earlier arguments [16, Proposition 2.2, Corollary 4.22] that rely on the screening parameter a being sufficiently small. Consequently, Propositions 2.5 and 2.6 are novel results as they guarantee the existence and uniqueness of the TFW Yukawa ground state for arbitrary values of a. $\square$

2.3 Preliminary results

The remainder of this chapter is dedicated to proving the main results on existence and uniqueness. We begin by showing several technical results which we will use make use of throughout the thesis.

Lemma 2.8. *Suppose $m : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$ and $m \in L^1_{\mathrm{loc}}(\mathbb{R}^3)$, then* (H2) *is equivalent to the following statement: there exist $\omega_0, \omega_1 > 0$ such that for all $R > 0$*

$$\inf_{x \in \mathbb{R}^3} \int_{B_R(x)} m(z) \, \mathrm{d}z \geq \omega_0 R^3 - \omega_1. \tag{2.8}$$

Proof of Lemma 2.8. Clearly, (2.8) implies (H2), so suppose m satisfies (H2), then there exists $R' > 0$ such that

$$\inf_{x \in \mathbb{R}^3} \int_{B_{R'}(x)} m(z) \, \mathrm{d}z \geq 1.$$

For $R > 0$ and $x' \in \mathbb{R}^3$, let $Q_R(x') \subset \mathbb{R}^3$ denote the cube of side length $2R$ centred at x', which contains $B_R(x')$. Also, let $R_0 = \frac{\sqrt{3}}{2} R'$ and $R = kR_0$, for $k \geq 1$. Then

$$\begin{aligned}
\inf_{x \in \mathbb{R}^3} \int_{B_R(x)} m(z) \, \mathrm{d}z \geq \inf_{x \in \mathbb{R}^3} \int_{Q_{kR'}(x)} m(z) \, \mathrm{d}z \geq \lfloor k \rfloor^3 \inf_{x' \in \mathbb{R}^3} \int_{Q_{R'}(x')} m(z) \, \mathrm{d}z \geq \lfloor k \rfloor^3 \\
\geq \left(\frac{k}{2} \right)^3 = \frac{R^3}{3\sqrt{3}(R')^3} =: \omega_0 R^3.
\end{aligned} \tag{2.9}$$

Now define $\omega_1 := \omega_0 R_0^3 \geq 0$, then it follows from (2.9) that (2.8) holds for all $R > 0$. $\square$

The following lemma features in the proofs of both the existence and uniqueness of the TFW equations and is found in [16, Page 93].

Lemma 2.9. *Let $f \in H^1_{\mathrm{loc}}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, then define the elliptic operator $L = -\Delta + f$. Suppose that there exists $u \in H^1_{\mathrm{loc}}(\mathbb{R}^3)$ satisfying $u > 0$ and*

$Lu = 0$ in the case of distributions. Then, the operator L is non-negative, that is

$$\langle \varphi, L\varphi \rangle \geq 0 \qquad \textit{for all} \;\; \varphi \in H^1(\mathbb{R}^3). \tag{2.10}$$

The proof is shown in [16, Page 93] but is included here for completeness.

Proof of Lemma 2.9. Let $R > 0$, define $\Omega = B_R(0)$ and consider $L = -\Delta + f$ as an operator acting on $H^1(\Omega)$ with Dirichlet boundary conditions. Then, since $f \in H^1_{\mathrm{loc}}(\mathbb{R}^3)$ it follows that the smallest eigenvalue $\lambda_1(\Omega)$ is simple and has a positive eigenfunction $v_\Omega \in H^1_0(\Omega)$ [28, Theorem 8.38]. In addition, by standard elliptic regularity $v_\Omega \in H^3(\Omega) \hookrightarrow C^{1,1/2}(\overline{\Omega})$ [24, Section 5.6.3, Theorem 6 and Section 6.3.2, Theorem 5] and solves

$$(-\Delta + f)\, v_\Omega = \lambda_1(\Omega) v_\Omega.$$

Testing this equation with u and using integration by parts, we obtain

$$-\int_{\partial\Omega} \frac{\partial v_\Omega}{\partial n} u = \lambda_1(\Omega) \int_\Omega v_\Omega u. \tag{2.11}$$

As $v_\Omega > 0$ on Ω and v_Ω vanishes over $\partial\Omega$, it follows that $\frac{\partial v_\Omega}{\partial n} \leq 0$. It follows that the left-hand side of (2.11) is non-negative, hence $\lambda_1(\Omega) \geq 0$. As this holds for $\Omega = B_R(0)$, for any $R > 0$, we deduce that for all $\varphi \in C^1_c(\mathbb{R}^3)$ $\langle \varphi, L\varphi \rangle \geq 0$. Using that $f \in L^\infty(\mathbb{R}^3)$ and the density of $C^1_c(\mathbb{R}^3)$ in $H^1(\mathbb{R}^3)$, it follows that for all $\varphi \in H^1(\mathbb{R}^3)$, $\langle \varphi, L\varphi \rangle \geq 0$. $\square$

The following technical lemma is used in the proofs of both existence and uniqueness for the Yukawa model.

Lemma 2.10. *Let $0 < a_1 \leq a_2$ and $m \in \mathcal{M}_{L^2}(M, \omega)$, then for $R_n > 0$ define $m_{R_n} = m \cdot \chi_{B_{R_n}(0)}$ and $\psi_{R_n} \in C^\infty_c(B_{4R_n}(0))$ satisfying $\psi_{R_n} \geq 0$, $\psi_{R_n} = 1$ on $B_{2R_n}(0)$ and $|\nabla \psi_{R_n}| \leq C R_n^{-1}$. Then there exists $C_0 = C_0(a_1, a_2, \omega) > 0$ and $R_0 = R_0(a_1, a_2, \omega) > 0$ such that for all $a_1 \leq a \leq a_2$ and $R_n \geq R_0$*

$$\int_{\mathbb{R}^3} |\nabla \psi_{R_n}|^2 - D_a(m_{R_n}, \psi^2_{R_n}) \leq -C_0 R_n^3. \tag{2.12}$$

Proof of Lemma 2.10. Let $a_1 \le a \le a_2$. By the construction of ψ_{R_n}

$$\int_{\mathbb{R}^3} |\nabla \psi_{R_n}|^2 = \int_{B_{4R_n}(0) \setminus B_{2R_n}(0)} |\nabla \psi_{R_n}|^2 \le C \int_{B_{4R_n}(0) \setminus B_{2R_n}(0)} R_n^{-2} \le C_1 R_n. \tag{2.13}$$

Additionally, it follows that

$$\begin{aligned} D_a(m_{R_n}, \psi_{R_n}^2) &= \int_{\mathbb{R}^3} (m_{R_n} * Y_a)\, \psi_{R_n}^2 \ge \int_{B_{2R_n}(0)} (m_{R_n} * Y_a)(x) \ \mathrm{d}x \\ &= \int_{\mathbb{R}^3} \left(\int_{B_{2R_n}(0) \cap B_{R_n}(y)} m_{R_n}(x-y) \ \mathrm{d}x \right) \frac{e^{-a|y|}}{|y|} \ \mathrm{d}y \\ &= \int_{\mathbb{R}^3} \left(\int_{B_{2R_n}(-y) \cap B_{R_n}(0)} m_{R_n}(x) \ \mathrm{d}x \right) \frac{e^{-a|y|}}{|y|} \ \mathrm{d}y. \end{aligned} \tag{2.14}$$

First consider for $R' > 0$

$$\int_{B_{R'}(0)} \frac{e^{-a|y|}}{|y|} \ \mathrm{d}y = 4\pi \int_0^{R'} r e^{-ar} \ \mathrm{d}r = \frac{4\pi}{a^2} \left(1 - e^{-aR'}(1 + aR') \right),$$

hence choosing $R' = (4a)^{-1}$ ensures that

$$\int_{B_{1/4a}(0)} \frac{e^{-a|y|}}{|y|} \ \mathrm{d}y = \frac{4\pi}{a^2} \left(1 - \tfrac{5}{4} e^{-1/4} \right) =: C_2 a^{-2},$$

where $C_2 > 0$. Now choose $R_n \ge (4a)^{-1}$, then the triangle inequality implies for $|y| \le (4a)^{-1}$, $B_{2R_n}(-y) \supset B_{R_n}(0)$, hence as $m \in \mathcal{M}_{L^2}(M, \omega)$

$$\int_{B_{2R_n}(-y) \cap B_{R_n}(0)} m_{R_n}(x) \ \mathrm{d}x \ge \int_{B_{R_n}(0)} m(x) \ \mathrm{d}x \ge \omega_0 R_n^3 - \omega_1. \tag{2.15}$$

Combining the inequalities (2.14)–(2.15) gives

$$\begin{aligned}
D_a(m_{R_n}, \psi_{R_n}^2) &= \int_{\mathbb{R}^3} \left(\int_{B_{2R_n}(-y)\cap B_{R_n}(0)} m_{R_n}(x)\,\mathrm{d}x \right) \frac{e^{-a|y|}}{|y|}\,\mathrm{d}y \\
&\geq \int_{B_{1/4a}(0)} \left(\int_{B_{2R_n}(-y)\cap B_{R_n}(0)} m_{R_n}(x)\,\mathrm{d}x \right) \frac{e^{-a|y|}}{|y|}\,\mathrm{d}y \\
&\geq \int_{B_{1/4a}(0)} \left(\int_{B_{R_n}(0)} m_{R_n}(x)\,\mathrm{d}x \right) \frac{e^{-a|y|}}{|y|}\,\mathrm{d}y \\
&\geq C_2 a^{-2}(\omega_0 R_n^3 - \omega_1). \qquad (2.16)
\end{aligned}$$

Now define $C_0 = \frac{C_2\omega_0}{2a_2^2} > 0$ and $R_n \geq R_0 := \max\{1, (4a_1)^{-1}, (\frac{C_1+C_2\omega_1 a_1^{-2}}{C_0})^{1/2}\}$, then combining (2.13) and (2.16) yields the desired estimate (2.12) for any $a_1 \leq a \leq a_2$ and $R_n \geq R_0$

$$\begin{aligned}
\int |\nabla\psi_{R_n}|^2 - D_a(m_{R_n}, \psi_{R_n}^2) &\leq \left(C_1 R_n + C_2\omega_1 a^{-2}\right) - 2C_0 R_n^3 \\
&\leq C_0 R_n^3 - 2C_0 R_n^3 = -C_0 R_n^3. \square
\end{aligned}$$

2.4 Proof of Coulomb existence and uniqueness

Our aim is to show Propositions 2.1, 2.2 and Corollary 2.3. The proof of Proposition 2.1 uses a thermodynamic limit argument, which involves showing uniform estimates for finite systems corresponding to nuclear distributions that are truncated over $B_R(0)$, then passing to the limit as $R \to \infty$. The following result is essentially [16, Proposition 3.5], however as we require uniform regularity estimates in the following chapters, we provide a complete proof.

Proposition 2.11. *Let $m : \mathbb{R} \to \mathbb{R}_{\geq 0}$ satisfy*

$$\|m\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq M, \qquad (2.17)$$

then for $R > 0$ define the truncated nuclear distribution $m_R = m \cdot \chi_{B_R(0)}$. There exists $R_0 > 0$ such that for all $R \geq R_0$, the unique solution to the *minimisation problem*

$$I^{\mathrm{TFW}}(m_R) = \inf \left\{ E^{\mathrm{TFW}}(v, m_R) \,\middle|\, v \in H^1(\mathbb{R}^3), v \geq 0, \int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m_R \right\} \tag{2.18}$$

yields the unique solution (u_R, ϕ_R) *to*

$$-\Delta u_R + \frac{5}{3} u_R^{7/3} - \phi_R u_R = 0, \tag{2.19a}$$

$$-\Delta \phi_R = 4\pi(m_R - u_R^2), \tag{2.19b}$$

which satisfy the following estimates, with constant C *independent of* R*:*

$$\|u_R\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(1 + M^{15/4}), \tag{2.20}$$

$$\|\phi_R\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(1 + M^{3/2}). \tag{2.21}$$

The charge constraint $\int_{\mathbb{R}^3} u_R^2 = \int_{\mathbb{R}^3} m_R$ in (2.18) ensures that when $m_R \not\equiv 0$, the corresponding electron density satisfies $u_R > 0$. It is also possible to consider the minimisation problem without imposing a charge constraint [47, Theorem 7.8].

Proof of Proposition 2.11. If $m \equiv 0$, then for all $R > 0$, clearly $u_R = \phi_R = 0$, $m_R = 0$ satisfy (2.19) and (2.20)–(2.21).

If $m \not\equiv 0$, then there exists a constant $R_0 \geq 0$ such that choosing $R \geq R_0$ ensures that $\int_{\mathbb{R}^3} m_R > 0$. Recall

$$E^{\mathrm{TFW}}(v, m_R) = \int_{\mathbb{R}^3} |\nabla v|^2 + \int_{\mathbb{R}^3} v^{10/3} + \frac{1}{2} D(m_R - v^2, m_R - v^2),$$

and the minimisation problem (2.18)

$$I^{\mathrm{TFW}}(m_R) = \inf \left\{ E^{\mathrm{TFW}}(v, m_R) \,\middle|\, v \in H^1(\mathbb{R}^3), v \geq 0, \int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m_R > 0 \right\}.$$

The constraint $\int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m_R > 0$ ensures the system is charge neutral, and by [47, Theorem 7.19] there exists a unique non-negative minimiser

$u_R \in H^1(\mathbb{R}^3)$ to $I^{\mathrm{TFW}}(m_R)$ solving

$$-\Delta u_R + \frac{5}{3} u_R^{7/3} - \left((m_R - u_R^2) * \tfrac{1}{|\cdot|} \right) u_R = -\theta_R u_R, \tag{2.22}$$

$$\int_{\mathbb{R}^3} u_R^2 = \int_{\mathbb{R}^3} m_R =: Z > 0. \tag{2.23}$$

Here $\theta_R \in \mathbb{R}$ is the Lagrange multiplier associated with the charge constraint (2.23).

We also consider the minimisation problem with the general charge constraint, for $\lambda \geq 0$

$$I^{\mathrm{TFW}}(m_R;\lambda) = \inf \left\{ E^{\mathrm{TFW}}(v, m_R) \,\middle|\, v \in H^1(\mathbb{R}^3), v \geq 0, \int_{\mathbb{R}^3} v^2 = \lambda \right\}. \tag{2.24}$$

By [47, Theorems 7.7, 7.8, 7.19], there exists a constant $\lambda_{\mathrm{c}} > Z$ such that $I^{\mathrm{TFW}}(m_R;\lambda)$ has a unique minimiser $u_{R,\lambda}$ if and only if $0 \leq \lambda \leq \lambda_{\mathrm{c}}$. When the minimiser $u_{R,\lambda}$ exists, it solves

$$-\Delta u_{R,\lambda} + \frac{5}{3} u_{R,\lambda}^{7/3} - \left((m_R - u_{R,\lambda}^2) * \tfrac{1}{|\cdot|} \right) u_{R,\lambda} = -\theta_{R,\lambda} u_{R,\lambda}, \tag{2.25}$$

where $\theta_{R,\lambda}$ is the associated Lagrange multiplier. In addition, $I^{\mathrm{TFW}}(m_R;\lambda)$ is decreasing in λ, $\theta_{R,\lambda} = -\frac{dI^{\mathrm{TFW}}(m_R;\lambda')}{d\lambda'}|_{\lambda'=\lambda}$ and $\lambda \mapsto \theta_{R,\lambda}$ is continuous. Consequently, for $\lambda \in [0, \lambda_{\mathrm{c}})$ it follows that $\theta_{R,\lambda} > 0$, hence $\theta_R = \theta_{R,Z} > 0$. Observe that $u_R = u_{R,Z}$ is the unique solution to (2.22).

For $\lambda \in [0, \lambda_{\mathrm{c}})$, define $\phi_{R,\lambda} : \mathbb{R}^3 \to \mathbb{R}$ by

$$\phi_{R,\lambda} = \left((m_R - u_{R,\lambda}^2) * \tfrac{1}{|\cdot|} \right) - \theta_{R,\lambda}, \tag{2.26}$$

so we can express (2.25) as the Schrödinger–Poisson system (2.19)

$$\begin{aligned} -\Delta u_{R,\lambda} + \frac{5}{3} u_{R,\lambda}^{7/3} - \phi_{R,\lambda} u_{R,\lambda} &= 0, \\ -\Delta \phi_{R,\lambda} &= 4\pi (m_R - u_{R,\lambda}^2). \end{aligned}$$

Decompose

$$(m_R - u_{R,\lambda}^2) * \tfrac{1}{|\cdot|} = (m_R - u_{R,\lambda}^2) * \left(\tfrac{1}{|\cdot|} \chi_{B_1(0)} \right) + (m_R - u_{R,\lambda}^2) * \left(\tfrac{1}{|\cdot|} \chi_{B_1(0)^{\mathrm{c}}} \right),$$

then by the Gagliardo–Nirenberg–Sobolev estimate [55, Theorem 2.2] $u_{R,\lambda} \in H^1(\mathbb{R}^3) \hookrightarrow L^6(\mathbb{R}^3)$ and as $m \in L^2_{\text{unif}}(\mathbb{R}^3)$, applying the Young inequality for convolutions gives

$$\begin{aligned}
\left\| (m_R - u_{R,\lambda}^2) * \tfrac{1}{|\cdot|} \right\|_{L^\infty(\mathbb{R}^3)} &\leq \|(m_R - u_{R,\lambda}^2)\|_{L^{5/3}(\mathbb{R}^3)} \left\| \tfrac{1}{|\cdot|} \chi_{B_1(0)} \right\|_{L^{5/2}(\mathbb{R}^3)} \\
&\quad + \|(m_R - u_{R,\lambda}^2)\|_{L^{7/5}(\mathbb{R}^3)} \left\| \tfrac{1}{|\cdot|} \chi_{B_1(0)^c} \right\|_{L^{7/2}(\mathbb{R}^3)} \\
&\leq C \left((R^{3/10} + R^{9/14}) \|m_R\|_{L^2(\mathbb{R}^3)} + \|u_{R,\lambda}\|^2_{H^1(\mathbb{R}^3)} \right) \\
&\leq C \left((R^{9/5} + R^{15/7}) \|m\|_{L^2_{\text{unif}}(\mathbb{R}^3)} + \|u_{R,\lambda}\|^2_{H^1(\mathbb{R}^3)} \right) \\
&\leq C \left((R^{9/5} + R^{15/7}) M + \|u_{R,\lambda}\|^2_{H^1(\mathbb{R}^3)} \right).
\end{aligned}$$

We make used of [46, Lemma II.25], which states that if $p, q \in (1, \infty)$ satisfy $\frac{1}{p} + \frac{1}{q} = 1$ and $f \in L^p(\mathbb{R}^3), g \in L^q(\mathbb{R}^3)$, then $f * g$ is a continuous function that converges to zero at infinity. Consequently, by applying [46, Lemma II.25] and the previous estimate, we deduce that $(m_R - u_{R,\lambda}^2) * \frac{1}{|\cdot|}$ is a continuous function vanishing at infinity. It follows that $\phi_{R,\lambda} \in L^\infty(\mathbb{R}^3)$ and is also continuous. Also, $|\nabla \phi_{R,\lambda}| \in L^2(\mathbb{R}^3)$,

$$\begin{aligned}
\frac{1}{8\pi} \int_{\mathbb{R}^3} |\nabla \phi_{R,\lambda}|^2 &= \frac{1}{8\pi} \int_{\mathbb{R}^3} \phi_{R,\lambda} \left(-\Delta \phi_{R,\lambda} \right) \\
&= \frac{1}{2} \int_{\mathbb{R}^3} \phi_{R,\lambda} (m_R - u_{R,\lambda}^2) \\
&= \frac{1}{2} \int_{\mathbb{R}^3} \phi_{R,\lambda} (m_R - u_{R,\lambda}^2) + \frac{\theta_{R,\lambda}}{2} \int_{\mathbb{R}^3} (m_R - u_{R,\lambda}^2) \\
&= \frac{1}{2} \int_{\mathbb{R}^3} \left(\phi_{R,\lambda} + \theta_{R,\lambda} \right) \left(m_R - u_{R,\lambda}^2 \right) \\
&= \frac{1}{2} \int_{\mathbb{R}^3} \left((m_R - u_{R,\lambda}^2) * \tfrac{1}{|\cdot|} \right) (m_R - u_{R,\lambda}^2),
\end{aligned} \tag{2.27}$$

hence $\phi_{R,\lambda} \in H^1_{\text{unif}}(\mathbb{R}^3)$. Moreover, as $\phi_{R,\lambda}$ solves $-\Delta \phi_{R,\lambda} = 4\pi(m_R - u_R^2)$ weakly and $m_R - u_R^2 \in L^2(\mathbb{R}^3)$, it follows from [24, Section 6.3.1, Theorem 1] that $\phi_{R,\lambda} \in H^2_{\text{unif}}(\mathbb{R}^3)$. Now, consider $u_{R,\lambda} \in H^1(\mathbb{R}^3)$, which solves

$$-\Delta u_{R,\lambda} = -\frac{5}{3} u_{R,\lambda}^{7/3} + \phi_{R,\lambda} u_{R,\lambda}. \tag{2.28}$$

The right-hand side can be estimated in $L^2(\mathbb{R}^3)$ by

$$\begin{aligned}\left\|\tfrac{5}{3}u_{R,\lambda}^{7/3}-\phi_{R,\lambda}u_{R,\lambda}\right\|_{L^2(\mathbb{R}^3)} &\leq \frac{5}{3}\left\|u_{R,\lambda}^{7/3}\right\|_{L^2(\mathbb{R}^3)}+\|\phi_{R,\lambda}\|_{L^\infty(\mathbb{R}^3)}\|u_{R,\lambda}\|_{L^2(\mathbb{R}^3)}\\ &\leq C\|u_{R,\lambda}\|_{H^1(\mathbb{R}^3)}^{7/3}+\|\phi_{R,\lambda}\|_{L^\infty(\mathbb{R}^3)}\|u_{R,\lambda}\|_{H^1(\mathbb{R}^3)},\end{aligned}$$

which implies $u_{R,\lambda} \in H^2(\mathbb{R}^3)$ as $\Delta u_{R,\lambda} \in L^2(\mathbb{R}^3)$. By the Sobolev Embedding Theorem [24, Section 5.6.3, Theorem 6] $u_{R,\lambda} \in H^2(\mathbb{R}^3) \hookrightarrow C^{0,1/2}(\mathbb{R}^3)$, thus $u_{R,\lambda}$ is continuous. We now justify that $u_{R,\lambda}$ decays at infinity by following the argument presented in [6, Lemma 9]. Recall (2.28) and since $u_{R,\lambda} \geq 0$, we have $-\Delta u_{R,\lambda} \leq \phi_{R,\lambda}u_{R,\lambda}$, hence

$$-\Delta u_{R,\lambda}+u_{R,\lambda} \leq (1+\phi_{R,\lambda})u_{R,\lambda}.$$

As $\phi_{R,\lambda} \in L^\infty(\mathbb{R}^3)$ and $u_{R,\lambda} \in H^1(\mathbb{R}^3)$, the right-hand side belongs to $L^2(\mathbb{R}^3)$ hence by the Lax-Milgram theorem there exists a unique $g_{R,\lambda} \in H^1(\mathbb{R}^3)$ satisfying

$$-\Delta g_{R,\lambda}+g_{R,\lambda} = (1+\phi_{R,\lambda})u_{R,\lambda}.$$

Moreover, using the Green's function $g_{R,\lambda} = \frac{e^{-|\cdot|}}{|\cdot|} * (1+\phi_{R,\lambda})u_{R,\lambda}$ and since $\frac{e^{-|\cdot|}}{|\cdot|}, (1+\phi_{R,\lambda})u_{R,\lambda} \in L^2(\mathbb{R}^3)$, by [46, Lemma II.25], $g_{R,\lambda}$ is a continuous function that decays at infinity, hence $g_{R,\lambda} \in L^\infty(\mathbb{R}^3)$. It follows from the comparison principle that $0 \leq u_{R,\lambda} \leq g_{R,\lambda}$, so $u_{R,\lambda} \in L^\infty(\mathbb{R}^3)$ and decays at infinity.

We now follow the argument of [62, Proposition 8] verbatim to show the Solovej estimate for $(u_R, \phi_R) = (u_{R,Z}, \phi_{R,Z})$,

$$\frac{10}{9}u_R^{4/3} \leq \phi_R + C_S. \tag{2.29}$$

For convenience, in the following argument $u_{R,\lambda}, \phi_{R,\lambda}, m_R, \theta_{R,\lambda}$ will be denoted as u, ϕ, m, θ. As u solves (2.19a)

$$-\Delta u + \frac{5}{3}u^{7/3} - \phi u = 0,$$

following the proof of [62, Proposition 8], $w = u^{4/3}$ is non-negative and satisfies

$$-\Delta w + \frac{4}{3}\left(\tfrac{5}{3}w - \phi\right) w \leq 0. \tag{2.30}$$

Let $\alpha \in (0, \frac{5}{3})$ and define

$$v = \alpha u^{4/3} - \phi - \theta - (C(\lambda) - \theta)_+,$$

where $C(\alpha) = (9/4)\pi^2\alpha^{-2}(\frac{5}{3} - \alpha)^{-1} > 0$. The equation (2.19b) can be written as

$$-\Delta\phi = 4\pi(m - w^{3/2}). \tag{2.31}$$

Combining (2.30) and (2.31), it follows that

$$\Delta v \geq \frac{4\alpha}{3}\left(\tfrac{5}{3}w - \phi\right) w - 4\pi w^{3/2} + 4\pi m.$$

The aim is to prove that $v \leq 0$ by showing that $S = \{x \,|\, v(x) > 0\}$ is empty. As u and $\phi + \theta$ are continuous functions that decay at infinity, it follows that v is continuous and converges to $-\theta - (C(\alpha) - \theta)_+ < 0$ at infinity, thus S is bounded, open and $v = 0$ on ∂S. Over S, using that $v > 0$, we deduce

$$\begin{aligned}
\Delta v &\geq \frac{4\alpha}{3}\left(v + \tfrac{5}{3}w - \alpha w + \theta + (C(\alpha) - \theta)_+\right) w - 4\pi w^{3/2} + 4\pi m \\
&\geq \frac{4\alpha}{3}\left(\tfrac{5}{3}w - \alpha w + C(\alpha)\right) w - 4\pi w^{3/2} + 4\pi m \\
&= \left(\frac{4\alpha(\frac{5}{3} - \alpha)}{3} w - 4\pi w^{1/2} + \frac{4\alpha}{3}C(\alpha)\right) w + 4\pi m.
\end{aligned}$$

The value of $C(\alpha)$ is chosen to ensure that

$$\frac{4\alpha(\frac{5}{3} - \alpha)}{3} w - 4\pi w^{1/2} + \frac{4\alpha}{3}C(\alpha) \geq 0,$$

hence as m is non-negative and $v > 0$ in S

$$\Delta v \geq 4\pi m \geq 0.$$

As v satisfies

$$\begin{aligned} -\Delta v &\leq 0 \quad \text{in } S, \\ v &= 0 \quad \text{on } \partial S, \end{aligned}$$

it follows that both $v \leq 0$ and $v > 0$ on S, hence S is empty and $v \leq 0$ on $\mathbb{R}^3$. So for all $\lambda \in [0, \lambda_c)$, $\alpha \in (0, \frac{5}{3})$ and all $x \in \mathbb{R}^3$

$$\alpha u_{R,\lambda}^{4/3}(x) \leq \phi_{R,\lambda}(x) + \theta_{R,\lambda} + (C(\alpha) - \theta_{R,\lambda})_+.$$

The right-hand side is minimised by choosing $\alpha = \frac{10}{9}$ and defining $C_S := C(\frac{10}{9})$, which gives

$$\frac{10}{9} u_{R,\lambda}^{4/3}(x) \leq \phi_{R,\lambda}(x) + \theta_{R,\lambda} + (C_S - \theta_{R,\lambda})_+. \tag{2.32}$$

In order to obtain the desired estimate (2.29), it remains to show that for $\lambda \in [Z, \lambda_c]$, we have $\theta_{R,\lambda} \leq C_S$.

We argue by contradiction, so first suppose that there exists $\lambda \in (Z, \lambda_c]$ such that $\theta_{R,\lambda} \geq C_S$, hence (2.32) implies

$$0 \leq \frac{10}{9} u_{R,\lambda}^{4/3} \leq \phi_{R,\lambda} + \theta_{R,\lambda} = (m_R - u_{R,\lambda}^2) * \tfrac{1}{|\cdot|}.$$

Observe that the minimiser $u_{R,\lambda}$ to $I^{\mathrm{TFW}}(m_R; \lambda)$ (2.24), satisfies $\int_{\mathbb{R}^3} u_{R,\lambda}^2 = \lambda > Z$, hence there exists $R_0 \geq R$ such that

$$\int_{B_{R_0}(0)} u_{R,\lambda}^2 - Z =: \varepsilon > 0. \tag{2.33}$$

Now let $|x| > R_0$, and recall that m_R is supported on $B_R(0) \subset B_{R_0}(0)$, so by applying the triangle inequality, we deduce

$$\left(m_R * \tfrac{1}{|\cdot|}\right)(x) = \int_{B_{R_0}(0)} \frac{m_R(y)}{|x-y|}\,\mathrm{d}y \leq \int_{B_{R_0}(0)} \frac{m_R(y)}{|x| - R_0}\,\mathrm{d}y = \frac{Z}{|x| - R_0}. \tag{2.34}$$

Similarly, using (2.33) we infer

$$\left(u_{R,\lambda}^2 * \tfrac{1}{|\cdot|}\right)(x) = \int_{\mathbb{R}^3} \frac{u_{R,\lambda}^2(y)}{|x-y|}\,\mathrm{d}y \geq \int_{B_{R_0}(0)} \frac{u^2(y)}{|x|+R_0}\,\mathrm{d}y = \frac{Z+\varepsilon}{|x|+R_0}. \tag{2.35}$$

Combining the estimates (2.34)–(2.35) gives

$$\left((m_R - u_{R,\lambda}^2) * \tfrac{1}{|\cdot|}\right)(x) \leq \frac{Z}{|x|-R_0} - \frac{Z+\varepsilon}{|x|+R_0} = \frac{(2Z+\varepsilon)R_0 - \varepsilon|x|}{|x|^2 - R_0^2},$$

hence choosing $|x| > \max\{R_0, (2Z+\varepsilon)\varepsilon^{-1}R_0\}$ gives the contradiction

$$0 \leq \left((m_R \ - \ u_{R,\lambda}^2) * \ \tfrac{1}{|\cdot|}\ \right)(x) \ < \ 0,$$

therefore, for all $\lambda \in (Z, \lambda_c]$, $\theta_{R,\lambda} < C_S$, hence as $\lambda \mapsto \theta_{R,\lambda}$ is continuous, it follows by sending $\lambda \searrow Z$ that $\theta_R = \theta_{R,Z} \leq C_S$, hence the desired estimate (2.32) holds.

As $u_R \geq 0$, from the Solovej estimate (2.29) we obtain the uniform lower bound

$$\phi_R \geq -C_S. \tag{2.36}$$

We aim to show a uniform upper bound for ϕ_R, which together with (2.29) will yield the uniform estimate

$$\|u_R\|_{L^\infty(\mathbb{R}^3)}^{4/3} + \|\phi_R\|_{L^\infty(\mathbb{R}^3)} \leq C(M), \tag{2.37}$$

which is independent of R.

If ϕ_R is non-positive, then (2.37) holds as

$$\|u_R\|_{L^\infty(\mathbb{R}^3)}^{4/3} + \|\phi_R\|_{L^\infty(\mathbb{R}^3)} \leq 2C_S.$$

Instead, suppose that $\phi_R^+ := \max\{\phi_R, 0\}$ is non-zero at some point in $\mathbb{R}^3$. By (2.26) ϕ_R is a continuous function that converges to a negative limit at infinity, $\phi_R^+ \in C_c(\mathbb{R}^3)$, hence there exists a point $x_R \in \mathbb{R}^3$ such that

$$\phi_R^+(x_R) = \|\phi_R^+\|_{L^\infty(\mathbb{R}^3)} > 0.$$

Without loss of generality, we assume $x_R = 0$, by translating m if necessary.

We now show that $u_R > 0$ on $\mathbb{R}^3$, arguing by contradiction. Suppose that there exists $z \in \mathbb{R}^3$ such that $u_R(z) = 0$. Since u_R is a non-negative, continuous function decaying at infinity, there exists $y \in \mathbb{R}^3$ such that

$$u_R(y) = \sup_{x \in \mathbb{R}^3} u_R(x),$$

so let $R' > |y - z|$. As $u_R \geq 0$ solves $L_R u_R = 0$, where $L_R = -\Delta + \frac{5}{3} u_R^{4/3} - \phi_R$, where $\frac{5}{3} u_R^{4/3} - \phi_R \in L^\infty(\mathbb{R}^3)$ and $u_R \in H^1(\mathbb{R}^3)$, then by the Harnack inequality [28, Theorem 8.20], we deduce

$$0 \leq u_R(y) = \sup_{x \in B_{R'}(y)} u_R(x) \leq C(R') \inf_{x \in B_{R'}(y)} u_R(x) = u_R(z) = 0, \tag{2.38}$$

so $u_R \equiv 0$. This contradicts the charge constraint (2.23) $\int_{\mathbb{R}^3} u_R^2 = \int_{\mathbb{R}^3} m_R > 0$, hence $u_R > 0$ on $\mathbb{R}^3$.

Consequently, as $u_R \in H^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3), \phi_R \in H^1_{\text{unif}}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ and $u_R > 0$, Lemma 2.9 implies that $L_R = -\Delta + \frac{5}{3} u_R^{4/3} - \phi_R$ is a non-negative operator.

Choose $\varphi \in C_c^\infty(B_1(0))$ satisfying $0 \leq \varphi \leq 1$, $\varphi = 1$ on $B_{1/2}(0)$, $\int_{\mathbb{R}^3} \varphi^2 = 1$ and $\int_{\mathbb{R}^3} |\nabla \varphi|^2 = c_\varphi$, then for $y \in \mathbb{R}^3$, define $\varphi_y \in C_c^\infty(B_1(y))$ by $\varphi_y = \varphi(\cdot - y)$. As L_R is non-negative (2.10) implies

$$\langle \varphi_y, L_R \varphi_y \rangle = \int_{\mathbb{R}^3} |\nabla \varphi_y|^2 + \int_{\mathbb{R}^3} \left(\frac{5}{3} u_R^{4/3} - \phi_R \right) \varphi_y^2 \geq 0,$$

which can be re-arranged and expressed using convolutions as

$$\begin{aligned} \frac{5}{3} \left(u_R^{4/3} * \varphi^2 \right) &\geq \left(\phi_R * \varphi^2 - \int_{\mathbb{R}^3} |\nabla \varphi|^2 \right)_+ \\ &= \left(\phi_R * \varphi^2 - c_\varphi \right)_+ . \end{aligned} \tag{2.39}$$

Observe that $\phi_R * \varphi^2$ solves

$$-\Delta \left(\phi_R * \varphi^2 \right) = 4\pi \left(m_R * \varphi^2 - u_R^2 * \varphi^2 \right). \tag{2.40}$$

We estimate the first term using (2.17)

$$
\begin{aligned}
4\pi\left(m_R*\varphi^2\right)(x) &= 4\pi\int_{B_1(x)} m_R(y)\varphi^2(x-y)\,\mathrm{d}y\\
&\le 4\pi\int_{B_1(x)} m(y)\,\mathrm{d}y \le C_0\|m\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \le C_0 M.
\end{aligned}
$$

For the second term, observe that as $\int_{\mathbb{R}^3}\varphi^2 = 1$, one can define the probability measure for Borel sets $A\subset\mathbb{R}^3$ by $\mu(A) = \int_A \varphi^2$. Using the convexity of $t\mapsto t^{3/2}$ and applying (2.39) and Jensen's inequality with μ, we deduce

$$
\begin{aligned}
4\pi\, u_R^2*\varphi^2(x) &\ge 4\pi u_R^2*\varphi^2(x)\\
&= 4\pi\int_{\mathbb{R}^3} u_R^2(x-y)\varphi^2(y)\,\mathrm{d}y\\
&= 4\pi\int_{\mathbb{R}^3}\left(u_R^{4/3}(x-y)\right)^{3/2}\varphi^2(y)\,\mathrm{d}y\\
&\ge 4\pi\left(\int_{\mathbb{R}^3} u_R^{4/3}(x-y)\varphi^2(y)\,\mathrm{d}y\right)^{3/2}\\
&= 4\pi(u_R^{4/3}*\varphi^2)^{3/2}\\
&\ge 4\pi\left(\frac{3}{5}\right)^{3/2}\left(\phi_R*\varphi^2-c_\varphi\right)_+^{3/2} \ge \left(\phi_R*\varphi^2-c_\varphi\right)_+^{3/2}. \qquad (2.41)
\end{aligned}
$$

Combining the estimates (2.40)–(2.41) we conclude that

$$
-\Delta\left(\phi_R*\varphi^2\right) + \left(\phi_R*\varphi^2-c_\varphi\right)_+^{3/2} \le C_0 M.
$$

By (2.26), as ϕ_R is a continuous function that converges to a negative limit at infinity, $\phi_R*\varphi^2$ also shares these properties. Define $f := \phi_R*\varphi^2 - c_\varphi$ and consider the set

$$
S = \{\, x\in\mathbb{R}^3 \mid f(x) > 0 \,\}.
$$

It follows that S is open and bounded and further that f satisfies

$$
\begin{aligned}
-\Delta f + f^{3/2} &\le C_0 M \quad \text{on } S, \qquad (2.42)\\
f &= 0 \quad \text{in } \partial S.
\end{aligned}
$$

Observe that the non-negative, constant function $g = (C_0 M)^{2/3}$ satisfies

$$-\Delta g + g^{3/2} = C_0 M \quad \text{on } S, \tag{2.43}$$
$$f \le g \quad \text{in } \partial S \cup S^{\mathrm{c}}. \tag{2.44}$$

We now show that $f \le g$ almost everywhere by a comparison principle argument. Consider the difference (2.42)–(2.43)

$$-\Delta(f-g) + f^{3/2} - g^{3/2} \le 0 \quad \text{on } S, \tag{2.45}$$

define $A := \{f > g\} \cap S \subseteq S$ and then test (2.45) by $(f-g)^+$ to obtain

$$\int_A \nabla(f-g)\cdot\nabla(f-g)^+ + \left(f^{3/2} - g^{3/2}\right)(f-g)^+ \le 0.$$

On A, it follows that $\nabla(f-g) = \nabla(f-g)^+$ and also by monotonicity $f^{3/2} - g^{3/2} > 0$, which implies

$$0 \le \int_A |\nabla(f-g)|^2 + \left(f^{3/2} - g^{3/2}\right)(f-g) \le 0.$$

Consequently, as $\left(f^{3/2} - g^{3/2}\right)(f-g) > 0$ on A, it follows that A is empty, so $f \le g$ almost everywhere on S, and also on S^{c} by (2.44), hence

$$\phi_R * \varphi^2 \le c_\varphi + (C_0 M)^{2/3} \le C(1 + M^{2/3}). \tag{2.46}$$

We now use (2.46) to construct an upper bound for ϕ_R^+, by applying the comparison principle once again. First, we require the following notation.

For a function $f : \mathbb{R}^3 \to \mathbb{R}$, define

$$\mathrm{sgn}(f)(x) = \begin{cases} \frac{f(x)}{|f(x)|}, & \text{when } f(x) \neq 0, \\ 0, & \text{otherwise,} \end{cases}$$

then as $\phi_R \in H^2_{\mathrm{unif}}(\mathbb{R}^3)$, Kato's inequality [37, Lemma A] implies that

$$-\Delta|\phi_R| \le \mathrm{sgn}(\phi_R)\,(-\Delta\phi_R) \quad \text{in distribution.}$$

We now show a similar estimate, that

$$-\Delta\phi_R^+ \le -\Delta\phi_R\chi_{\{\phi_R>0\}} \quad \text{in distribution,} \tag{2.47}$$

i.e. for all $\varphi \in C_c^\infty(\mathbb{R}^3)$ satisfying $\varphi \ge 0$, we have

$$\int_{\mathbb{R}^3} \phi_R^+(-\Delta\varphi) \le \int_{\{\phi_R>0\}} (-\Delta\phi_R)\,\varphi.$$

We provide a justification of (2.47), following the proof of [37, Lemma A]. For $f : \mathbb{R}^3 \to \mathbb{R}$ and $\varepsilon > 0$, let $f_\varepsilon = (f^3 + \varepsilon^3)^{1/2}$ and $f_\varepsilon^+ = \max\{f_\varepsilon - \varepsilon, 0\}$. As $f \in C^2(\mathbb{R}^3)$ implies $f_\varepsilon^+ := (f_\varepsilon)^+ \in C^2(\mathbb{R}^3)$, a direct calculation shows that over $\{f > 0\}$

$$\Delta f_\varepsilon^+ = \frac{f^2}{(f_\varepsilon)^2}\Delta f + 2\varepsilon^3\frac{f|\nabla f|^2}{(f_\varepsilon)^5} \ge \frac{f^2}{(f_\varepsilon)^2}\Delta f.$$

It follows that

$$\Delta f_\varepsilon^+ \ge \begin{cases} \frac{f^2}{(f_\varepsilon)^2}\Delta f & \text{on } \{f>0\}, \\ 0 & \text{otherwise,} \end{cases}$$

hence $\Delta(f_\varepsilon)^+ \ge \frac{f^2}{(f_\varepsilon)^2}(\Delta f)\chi_{\{f>0\}}$.

For $f \in H^2_{\text{unif}}(\mathbb{R}^3)$, choose $\eta \in C_c^\infty(B_1(0))$ satisfying $\eta \ge 0$ and $\int \eta = 1$, then for $\delta > 0$, define $\eta(x) = \delta^{-3}\eta(\frac{x}{\delta})$ and $f^\delta := f * \eta_\delta$. It follows that $f^\delta \to f$ in $H^2_{\text{unif}}(\mathbb{R}^3)$ and pointwise almost everywhere.

Now for $\varepsilon, \delta > 0$, define $f_\varepsilon^\delta := (f_\varepsilon)^\delta$ which satisfies $f_\varepsilon^\delta \to f_\varepsilon$ in $H^2_{\text{unif}}(\mathbb{R}^3)$ and pointwise almost everywhere. In particular $\Delta(f_\varepsilon^\delta)^+ \ge \frac{(f^\delta)^2}{(f_\varepsilon^\delta)^2}(\Delta f^\delta)\chi_{\{f^\delta>0\}}$, so we pass to the limit in distribution as $\delta \to 0$, for fixed ε. As $\Delta f_\varepsilon^\delta \to \Delta f_\varepsilon$ in $L^2_{\text{unif}}(\mathbb{R}^3)$, it follows that $\Delta f_\varepsilon^\delta \to \Delta f_\varepsilon$ in distribution as $\delta \to 0$. Since $\text{spt}(\eta_\delta) \subset B_\delta(0)$, it follows that $\chi_{\{f^\delta>0\}} \to \chi_{\{f>0\}}$ pointwise almost everywhere, so $\frac{(f^\delta)^2}{(f_\varepsilon^\delta)^2}\chi_{\{f^\delta>0\}} \to \frac{f^2}{(f_\varepsilon)^2}\chi_{\{f>0\}}$ pointwise almost everywhere as $\delta \to 0$. For

$\varphi \in C_c^\infty(\mathbb{R}^3)$ satisfying $\varphi \geq 0$,

$$
\begin{aligned}
&\left| \int_{\mathbb{R}^3} \left(\frac{(f^\delta)^2}{(f_\varepsilon^\delta)^2} \chi_{\{f^\delta > 0\}} (\Delta f^\delta) - \frac{f^2}{(f_\varepsilon)^2} \chi_{\{f>0\}} (\Delta f) \right) \varphi \right| \\
&\qquad \leq \int_{\mathbb{R}^3} \left| \frac{(f^\delta)^2}{(f_\varepsilon^\delta)^2} \chi_{\{f^\delta > 0\}} - \frac{f^2}{(f_\varepsilon)^2} \chi_{\{f>0\}} \right| |\Delta f| |\varphi| \\
&\qquad\quad + \int_{\mathbb{R}^3} \left| \frac{(f^\delta)^2}{(f_\varepsilon^\delta)^2} \chi_{\{f^\delta > 0\}} \right| |\Delta f^\delta - \Delta f| |\varphi| \\
&\qquad \leq \int_{\mathbb{R}^3} \left| \frac{(f^\delta)^2}{(f_\varepsilon^\delta)^2} \chi_{\{f^\delta > 0\}} - \frac{f^2}{(f_\varepsilon)^2} \chi_{\{f>0\}} \right| |\Delta f| |\varphi| + \int_{\mathbb{R}^3} |\Delta f^\delta - \Delta f| |\varphi|,
\end{aligned}
$$

which tends to 0 as $\delta \to 0$ by applying the Dominated Convergence Theorem. It follows that

$$
\Delta f_\varepsilon^+ \geq \frac{f^2}{(f_\varepsilon)^2} (\Delta f) \chi_{\{f>0\}} \quad \text{in distribution.} \tag{2.48}
$$

We now pass to the limit in (2.48) by sending $\varepsilon \to 0$. As f_ε converges absolutely to f^+ and $\frac{f}{f_\varepsilon} \chi_{\{f>0\}} \to \chi_{\{f>0\}}$ pointwise almost everywhere as $\varepsilon \to 0$, it follows that $\Delta f_\varepsilon^+ \to \Delta f^+$ and $\frac{f^2}{(f_\varepsilon)^2} (\Delta f) \chi_{\{f>0\}} \to (\Delta f) \chi_{\{f>0\}}$ in distribution, hence sending $\varepsilon \to 0$ in (2.48) yields the desired estimate

$$
\Delta f^+ \geq (\Delta f) \chi_{\{f>0\}} \quad \text{in distribution,}
$$

which proves (2.47).

Now recall (2.19b), that $-\Delta \phi_R = 4\pi(m_R - u_R^2)$, we then deduce that

$$
-\Delta \phi_R^+ \leq (-\Delta \phi_R) \chi_{\{\phi_R > 0\}} = 4\pi \left(m_R - u_R^2 \right) \chi_{\{\phi_R > 0\}} \leq 4\pi m_R \leq 4\pi m, \tag{2.49}
$$

in distribution. We now show that (2.49) can be extended to show that for all $v \in H^1(K)$, where $K \subset \mathbb{R}^3$ is bounded, satisfying $v \geq 0$, we have

$$
\int_K \nabla \phi_R^+ \cdot \nabla v \leq 4\pi \int_K m v. \tag{2.50}
$$

This is required to show a maximum principle estimate for ϕ_R^+. Given $v \in H^1(K)$, where $v \geq 0$ and $K \subset \mathbb{R}^3$ is bounded, for $\delta > 0$ define the smooth approximation v^δ using the construction specified on Page 34, which ensures that $v^\delta \geq 0$ for all $\delta > 0$. Let $K' \supset K$, there exists $\delta_0 > 0$ such that for all $0 < \delta \leq \delta_0$, we have $v^\delta \in C_c^\infty(K')$ and further $v^\delta \to v$ in $H^1(K')$ as $\delta \to 0$. As $\phi_R \in H^2_{\mathrm{unif}}(\mathbb{R}^3)$, applying [45, Theorem 6.17] gives that $\phi_R^+ \in H^1_{\mathrm{unif}}(\mathbb{R}^3)$ and $\nabla\phi_R^+ = \nabla\phi_R\chi_{\{\phi_R>0\}}$. For $0 < \delta \leq \delta_0$, applying (2.49) gives

$$\int_{K'} \nabla\phi_R^+ \cdot \nabla v^\delta = \int_{K'} \phi_R^+(-\Delta v^\delta) \leq 4\pi \int_{K'} m v^\delta, \tag{2.51}$$

then using that $m \in L^2_{\mathrm{unif}}(\mathbb{R}^3)$ and $v^\delta \to v$ in $H^1(K')$, passing to the limit in (2.51) as $\delta \to 0$ yields the desired estimate (2.50)

$$\int_K \nabla\phi_R^+ \cdot \nabla v \leq 4\pi \int_K mv.$$

We now apply (2.46) and the lower bound (2.36), $\phi_R \geq -C_S$, to show

$$\phi_R^+ * \varphi^2 = \phi_R^- * \varphi^2 + \phi_R * \varphi^2 \leq C_S + C(1 + M^{2/3}) = C(1 + M^{2/3}),$$

using that $\int_{\mathbb{R}^3} \varphi^2 = 1$. As $0 \leq \varphi \leq 1$ and $\varphi = 1$ on $B_{1/2}(0)$, then

$$\int_{B_{1/2}(0)} \phi_R^+(x)\,\mathrm{d}x \leq \left(\phi_R^+ * \varphi^2\right)(0) \leq C(1 + M^{2/3}). \tag{2.52}$$

For $r > 0$, let $d\sigma_r$ denote the spherical measure over the sphere $S_r := \partial B_r(0)$, then using a change of variables, (2.52) can be expressed as

$$\begin{aligned}\int_{B_{1/2}(0)} \phi_R^+(x)\,\mathrm{d}x &= \int_0^{1/2} r^2 \int_{S_1} \phi_R^+(rz)\,\mathrm{d}\sigma_1(z)\,\mathrm{d}r \\ &= \int_0^{1/2} \int_{S_r} \phi_R^+(y)\,\mathrm{d}\sigma_r(y)\,\mathrm{d}r.\end{aligned}$$

Define $f : (0, 1/2] \to \mathbb{R}$ by

$$f(r) = \int_{S_r} \phi_R^+(y)\,\mathrm{d}\sigma_r(y).$$

We suppose that for all $r \in (1/4, 1/2)$

$$f(r) > 4 \int_{B_{1/2}(0)} \phi_R^+(x)\ \mathrm{d}x > 0,$$

then

$$\int_{B_{1/2}(0)} \phi_R^+(x)\ \mathrm{d}x = \int_0^{1/2} f(r)\ \mathrm{d}r \geq \int_{1/4}^{1/2} f(r)\ \mathrm{d}r > \int_{B_{1/2}(0)} \phi_R^+(x)\ \mathrm{d}x,$$

which gives a contradiction, hence for some $r_0 \in (1/4, 1/2)$

$$f(r_0) = \int_{S_{r_0}} \phi_R^+(y)\ \mathrm{d}\sigma_{r_0}(y) \leq 4 \int_{B_{1/2}(0)} \phi_R^+(x)\ \mathrm{d}x \leq C(1 + M^{2/3}). \tag{2.53}$$

Since $r_0 > 1/4$, (2.53) implies

$$\begin{aligned} \fint_{S_{r_0}} \phi_R^+(y)\ \mathrm{d}\sigma_{r_0}(y) &= \frac{1}{|S_{r_0}|} \int_{S_{r_0}} \phi_R^+(y)\ \mathrm{d}\sigma_{r_0}(y) \\ &\leq \frac{C(1 + M^{2/3})}{|S_{1/4}|} =: C_1(M). \end{aligned}$$

We now construct an upper bound for ϕ_R^+ as follows. Let ϕ_1 satisfy

$$\begin{aligned} -\Delta \phi_1 &= 0 \qquad \text{in } B_{r_0}(0), \\ \phi_1 &= \phi_R^+ \quad \text{on } S_{r_0}. \end{aligned}$$

As ϕ_1 is harmonic, it satisfies the mean value property

$$\phi_1(0) = \fint_{S_r} \phi_1(y)\ \mathrm{d}\sigma_{r_0}(y) = \fint_{S_r} \phi_R^+(y)\ \mathrm{d}\sigma_{r_0}(y) \leq C_1(M). \tag{2.54}$$

Then consider the Dirichlet problem

$$\begin{aligned} -\Delta \phi_2 &= 4\pi m \quad \text{in } B_{r_0}(0), \\ \phi_2 &= 0 \qquad \text{on } S_{r_0}. \end{aligned}$$

By Lax-Milgram, this has a unique weak solution $\phi_2 \in H_0^1(B_{r_0}(0))$. By standard elliptic regularity theory [24, Section 5.6.3, Theorem 6], we have

$\phi_2 \in H^2(B_{r_0}(0)) \hookrightarrow C^{0,1/2}(\overline{B_{r_0}(0)})$ and

$$\begin{aligned}\|\phi_2\|_{C^{0,1/2}(\overline{B_{r_0}(0)})} &\leq C\|\phi_2\|_{H^2(B_{r_0}(0))} \leq C\|m\|_{L^2(B_{r_0}(0))} \\ &\leq Cr_0^{3/2}\|m\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq CM. \end{aligned} \tag{2.55}$$

The constructed functions ϕ_1, ϕ_2 satisfy

$$\begin{aligned} -\Delta\phi_R^+ &\leq -\Delta(\phi_1+\phi_2) \quad && \text{in } B_t(0), \\ \phi_R^+ &= \phi_1+\phi_2 && \text{on } S_t(0), \end{aligned}$$

hence applying (2.50) and the maximum principle argument shown on Page 32, we deduce $\phi_R^+ \leq \phi_1 + \phi_2$, in particular (2.54)–(2.55) imply

$$\|\phi_R^+\|_{L^\infty(\mathbb{R}^3)} = \phi_R^+(0) \leq \phi_1(0) + \phi_2(0) \leq C(1+M),$$

where the right-hand side is independent of R. Combining this with the lower bound (2.36) and the Solovej estimate (2.29), we obtain the estimate (2.37)

$$\|u_R\|_{L^\infty(\mathbb{R}^3)}^{4/3} + \|\phi_R\|_{L^\infty(\mathbb{R}^3)} \leq C(1+M).$$

It follows immediately that for all $x \in \mathbb{R}^3$ and $p \in [1,\infty]$

$$\|u_R\|_{L^p(B_2(x))} \leq C(1+M^{3/4}), \tag{2.56}$$

independently of both x, p and R. Using (2.37) and (2.56), we now obtain uniform local estimates for the right-hand side of (2.28)

$$-\Delta u_R = -\frac{5}{3}u_R^{7/3} + \phi_R u_R$$

by

$$\begin{aligned}\|\tfrac{5}{3}u_R^{7/3} - \phi_R u_R\|_{L^2(B_2(x))} &\leq C\|\tfrac{5}{3}u_R^{7/3} - \phi_R u_R\|_{L^\infty(\mathbb{R}^3)} \\ &\leq C(\|u_R\|_{L^\infty(\mathbb{R}^3)}^{7/3} + \|\phi_R\|_{L^\infty(\mathbb{R}^3)}\|u_R\|_{L^\infty(\mathbb{R}^3)}) \\ &\leq C(1+M^{7/4}).\end{aligned}$$

Consequently, for any $x \in \mathbb{R}^3$, the elliptic regularity estimate [24, Section 6.3.1, Theorem 1] gives

$$\begin{aligned}\|u_R\|_{H^2(B_1(x))} &\leq C(\|\tfrac{5}{3}u_R^{7/3} - \phi_R u_R\|_{L^2(B_2(x))} + \|u_R\|_{L^2(B_2(x))}) \\ &\leq C(1 + M^{7/4}) + C(1 + M^{1/2}) \leq C(1 + M^{7/4}). \qquad (2.57)\end{aligned}$$

As (2.57) is independent of $x \in \mathbb{R}^3$, we obtain

$$\|u_R\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(1 + M^{7/4}). \qquad (2.58)$$

Applying a similar argument to estimate the right-hand side of (2.19b)

$$-\Delta\phi_R = 4\pi(m_R - u_R^2)$$

yields (2.21),

$$\|\phi_R\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(1 + M^{3/2}).$$

Using that $\phi_R \in H^2_{\mathrm{unif}}(\mathbb{R}^3)$ and arguing as in (2.58), we obtain the desired estimate (2.20)

$$\|u_R\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(1 + M^{15/4}). \qquad \square$$

We now prove Proposition 2.1 by passing to the limit in (2.19).

Proof of Proposition 2.1. First suppose that $\mathrm{spt}(m)$ is bounded, then for sufficiently large R_n, $m = m_{R_n}$ and hence by Proposition 2.11 $(u, \phi) = (u_{R_n}, \phi_{R_n})$ solves (2.2) and satisfies the desired estimates (2.5)–(2.6).

Now suppose $\mathrm{spt}(m)$ is unbounded, then the estimates (2.20)–(2.21) of Proposition 2.11 guarantee that the sequences u_{R_n}, ϕ_{R_n} are bounded uniformly in $H^2_{\mathrm{unif}}(\mathbb{R}^3)$. Consequently, there exist $u, \phi \in H^2_{\mathrm{unif}}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ such that along a subsequence u_{R_n}, ϕ_{R_n} converges to u, ϕ, weakly in $H^2(B_R(0))$, strongly in $H^1(B_R(0))$ for all $R > 0$ and pointwise almost everywhere. It follows from the pointwise convergence that $u \geq 0$ and

$$\|u\|_{L^\infty(\mathbb{R}^3)} \leq C(1 + M^{3/4}), \qquad (2.59)$$

$$\|\phi\|_{L^\infty(\mathbb{R}^3)} \leq C(1 + M). \qquad (2.60)$$

We now show that passing to the limit of the equations (2.19) in the sense of distributions yields

$$
\begin{aligned}
-\Delta u + \frac{5}{3}u^{7/3} - \phi u = 0, \\
-\Delta \phi = 4\pi(m - u^2).
\end{aligned}
$$

Let $\varphi \in C_c^\infty(\mathbb{R}^3)$, hence there exists $R' > 0$ such that $\operatorname{spt}(\varphi) \subset B_{R'}(0)$. For $p \geq 1$, applying Mean Value Theorem and (2.37), (2.59) implies there exists $\theta \in (0,1)$

$$
\begin{aligned}
|u_{R_n}^p - u^p| &= p| \left(\theta u_{R_n} + (1-\theta)u\right)^{p-1} ||u_{R_n} - u| \\
&\leq p\left(\|u_{R_n}\|_{L^\infty(\mathbb{R}^3)} + \|u\|_{L^\infty(\mathbb{R}^3)}\right)^{p-1} |u_{R_n} - u| \leq C|u_{R_n} - u|.
\end{aligned}
$$

It follows that

$$
\begin{aligned}
\left|\int_{\mathbb{R}^3} \left(u_{R_n}^p - u^p\right)\varphi\right| &\leq \int_{B_{R'}(0)} |u_{R_n}^p - u^p||\varphi| \leq C\int_{B_{R'}(0)} |u_{R_n} - u||\varphi| \\
&\leq \|u_{R_n} - u\|_{L^2(B_{R'}(0))}\|\varphi\|_{L^2(B_{R'}(0))} \to 0 \quad \text{as } R_n \to \infty.
\end{aligned}
$$

Similarly, by applying (2.37) and (2.59)–(2.60), we deduce

$$
\begin{aligned}
&\left|\int_{\mathbb{R}^3} (\phi_{R_n}u_{R_n} - \phi u)\varphi\right| \leq \int_{B_{R'}(0)} |\phi_{R_n} - \phi||u_{R_n}||\varphi| + \int_{B_{R'}(0)} |u_{R_n} - u||\phi||\varphi| \\
&\leq \left(\|u_{R_n}\|_{L^\infty(\mathbb{R}^3)}\|\phi_{R_n} - \phi\|_{L^2(B_{R'}(0))} + \|\phi\|_{L^\infty(\mathbb{R}^3)}\|u_{R_n} - u\|_{L^2(B_{R'}(0))}\right)\|\varphi\|_{L^2(B_{R'}(0))} \\
&\leq C\left(\|\phi_{R_n} - \phi\|_{L^2(B_{R'}(0))} + \|u_{R_n} - u\|_{L^2(B_{R'}(0))}\right) \to 0 \quad \text{as } R_n \to \infty.
\end{aligned}
$$

In addition, choosing $R_n \geq R'$ ensures that

$$
\int_{B_{R'}(0)} m_{R_n}\varphi = \int_{B_{R'}(0)} m\varphi,
$$

and a straightforwards application of integration by parts shows that $\lim_{R_n\to\infty}\int_{\mathbb{R}^3} -\Delta u_{R_n}\varphi = \int_{\mathbb{R}^3} -\Delta u\varphi, \lim_{R_n\to\infty}\int_{\mathbb{R}^3} -\Delta\phi$, hence (u,ϕ) solves (2.2) in the sense of distributions. Arguing as in (2.20)–(2.21), we deduce that the desired estimates (2.5)–(2.6) hold

$$\|u\|_{H^4_{\text{unif}}(\mathbb{R}^3)} \le C(1+M^{15/4}),$$

$$\|\phi\|_{H^2_{\text{unif}}(\mathbb{R}^3)} \le C(1+M^{3/2}). \qquad \square$$

Next, we prove the uniqueness result Proposition 2.2.

Proof of Proposition 2.2. As $m \in \mathcal{M}_{L^2}(M,\omega)$, it satisfies (H1)–(H2), hence by [16, Theorem 6.10], the solution (u,ϕ) of (2.2) defined in Proposition 2.1 is unique and satisfies $\inf u > 0$. Now suppose

$$\inf_{m \in \mathcal{M}_{L^2}(M,\omega)} \inf_{x \in \mathbb{R}^3} u(x) = 0. \tag{2.61}$$

We will show that this contradicts the assumption that for all $m \in \mathcal{M}_{L^2}(M,\omega)$ and $R > 0$

$$\inf_{x\in\mathbb{R}^3} \int_{B_R(x)} m(z)\,\mathrm{d}z \ge \omega_0 R^3 - \omega_1.$$

It follows from (2.61) that there exists $m_n \in \mathcal{M}_{L^2}(M,\omega)$ with corresponding solution (u_n,ϕ_n) and $x_n \in \mathbb{R}^3$ such that for all $n \in \mathbb{N}$

$$u_n(x_n) \le \frac{1}{n}.$$

Recall the uniform estimates (2.20)–(2.21) from Proposition 2.1

$$\|u_n\|_{H^4_{\text{unif}}(\mathbb{R}^3)} \le C(1+M^{15/4}),$$
$$\|\phi_n\|_{H^2_{\text{unif}}(\mathbb{R}^3)} \le C(1+M^{3/2}).$$

It follows that

$$\left\|\tfrac{5}{3}u_n^{4/3} - \phi_n u_n\right\|_{L^\infty(\mathbb{R}^3)} \le C\|u_n\|^{4/3}_{L^\infty(\mathbb{R}^3)} + \|\phi_n\|_{L^\infty(\mathbb{R}^3)} \le C(M), \tag{2.62}$$

where the constant is independent of $n \in \mathbb{N}$. As $\frac{5}{3}u_n^{4/3} - \phi_n \in L^\infty(\mathbb{R}^3)$,

$u_n \in H^1_{\text{unif}}(\mathbb{R}^3)$ and $u_n > 0$ solves

$$L_n u_n := \left(-\Delta + \frac{5}{3}u_n^{4/3} - \phi_n\right) u_n = 0,$$

applying the Harnack inequality [28, Theorem 8.20], and observing that the coefficients of L_n are uniformly estimated by (2.62), we deduce that for all $R > 0$, there exists $C = C(R, M) > 0$, independent of $n \in \mathbb{N}$, such that

$$\sup_{x \in B_R(x_n)} u_n(x) \leq C \inf_{x \in B_R(x_n)} u_n(x) \leq \frac{C}{n}.$$

It follows that the sequence of functions $u_n(\cdot + x_n)$ converges uniformly to zero on compact sets. Consider the ground state (u_n, ϕ_n) corresponding to the nuclear distribution m_n.

Recall that ϕ_n solves the following equation in the sense of distributions

$$-\Delta \phi_n = 4\pi \left(m_n - u_n^2\right). \tag{2.63}$$

We translate the system and then pass to the limit in (2.63) as n tends to infinity. To do this, we use the following estimates, which are translation invariant:

$$\|m_n(\cdot + x_n)\|_{L^2_{\text{unif}}(\mathbb{R}^3)} \leq M,$$
$$\|\phi_n(\cdot + x_n)\|_{H^2_{\text{unif}}(\mathbb{R}^3)} \leq C(M).$$

It follows that, up to a subsequence, $\phi_n(\cdot + x_n)$ converges to $\widetilde{\phi}$, weakly in $H^2(B_R(0))$, strongly in $H^1(B_R(0))$ for all $R > 0$ and pointwise almost everywhere. Moreover, $m_n(\cdot + x_n)$ converges to $\widetilde{m}$, weakly in $L^2(B_R(0))$ for all $R > 0$. It follows that

$$\|\widetilde{m}\|_{L^2_{\text{unif}}(\mathbb{R}^3)} = \sup_{x \in \mathbb{R}^3} \|\widetilde{m}\|_{L^2(B_1(x))} \leq \sup_{x \in \mathbb{R}^3} \liminf_{n \to \infty} \|m_n\|_{L^2(B_1(x))} \leq M, \tag{2.64}$$

and for all $R > 0$ and $x \in \mathbb{R}^3$

$$\int_{B_R(x)} \widetilde{m}(z)\, \mathrm{d}z = \lim_{n \to \infty} \int_{B_R(x)} m_n(z)\, \mathrm{d}z \geq \omega_0 R^3 - \omega_1, \tag{2.65}$$

hence $\widetilde{m} \in \mathcal{M}_{L^2}(M, \omega)$. Passing to the limit in

$$-\Delta\phi_n(\cdot + x_n) = 4\pi \left(m_n(\cdot + x_n) - u_n^2(\cdot + x_n) \right),$$

it follows that $\widetilde{\phi}$ is a distributional solution of

$$-\Delta\widetilde{\phi} = 4\pi\widetilde{m}. \tag{2.66}$$

We now show that (2.66) leads to a contradiction, as it implies for all $R > 0$

$$\int_{B_R(0)} \widetilde{m}(z) \, \mathrm{d}z \leq CR. \tag{2.67}$$

As $\widetilde{m} \in \mathcal{M}_{L^2}(M, \omega)$, this leads to the contradiction that for all $R > 0$

$$\omega_0 R^3 - \omega_1 \leq \int_{B_R(0)} \widetilde{m}(z) \, \mathrm{d}z \leq CR.$$

To show (2.67) choose $\varphi \in C_{\mathrm{c}}^{\infty}(B_2(0))$ such that $0 \leq \varphi \leq 1$ and $\varphi = 1$ on $B_1(0)$. Let $R > 0$, then testing (2.66) with $\varphi(\cdot/R)$ gives

$$-\frac{1}{R^2} \int_{B_{2R}(0)} \widetilde{\phi}(z)(\Delta\varphi)(z/R) \, \mathrm{d}z = 4\pi \int_{B_{2R}(0)} \widetilde{m}(z)\varphi(z/R) \, \mathrm{d}z. \tag{2.68}$$

The left-hand side can be estimated by

$$\frac{1}{R^2} \left| \int_{B_{2R}(0)} \widetilde{\phi}(z)(\Delta\varphi)(z/R) \, \mathrm{d}z \right| \leq \|\widetilde{\phi}\|_{L^\infty(\mathbb{R}^3)} \|\Delta\varphi\|_{L^\infty(\mathbb{R}^3)} \frac{|B_{2R}(0)|}{R^2} \leq CR,$$

where the constant $C > 0$ is independent of R. As $\widetilde{m} \geq 0$, from (2.68) we obtain (2.67)

$$\int_{B_R(0)} \widetilde{m}(z) \, \mathrm{d}z \leq \int_{B_{2R}(0)} \widetilde{m}(z)\varphi(z/R) \, \mathrm{d}z \leq CR.$$

The contradiction ensures that there exists a constant $c_{M,\omega} > 0$ such that for all $m \in \mathcal{M}_{L^2}(M, \omega)$, the corresponding electron density u satisfies

$$\inf_{x \in \mathbb{R}^3} u(x) \geq c_{M,\omega} > 0. \qquad \square$$

Proof of Corollary 2.3. Our aim is to show by induction that for all $k \in \mathbb{N}_0$, if $m \in \mathcal{M}_{H^k}(M,\omega)$ then the corresponding solution (u,ϕ) to (2.2) satisfies

$$\|u\|_{H^{k+4}_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi\|_{H^{k+2}_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(k,M,\omega). \tag{2.69}$$

In Proposition 2.1, by combining the estimates (2.5) and (2.6), it follows that (2.69) holds for the case $k=0$: for all $m \in \mathcal{M}_{L^2}(M,\omega)$ the corresponding solution (u,ϕ) satisfies

$$\|u\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M,\omega).$$

We now show the induction step. Suppose the result is true for $k \in \mathbb{N}_0$, then consider $m \in \mathcal{M}_{H^{k+1}}(M,\omega) \subset \mathcal{M}_{H^k}(M,\omega)$, so by the induction hypothesis the corresponding solution (u,ϕ) satisfies

$$\|u\|_{H^{k+4}_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi\|_{H^{k+2}_{\mathrm{unif}}(\mathbb{R}^3)} \leq C\left(k, \|m\|_{H^k_{\mathrm{unif}}(\mathbb{R}^3)}, \omega\right).$$

Applying Propositions 2.1 and 2.2 we obtain that $0 < c_{M,\omega} \leq u \leq C(M)$, hence for all $r \in \mathbb{R}$

$$\|u^r\|_{L^\infty(\mathbb{R}^3)} \leq c_{M,\omega}^{-r}\chi_{\{r<0\}} + \chi_{\{r=0\}} + C(M)^r\chi_{\{r>0\}} =: \widetilde{C}(r,M,\omega)$$

We now show that for all $p \in \mathbb{R}$, $u^p \in H^{k+3}_{\mathrm{unif}}(\mathbb{R}^3)$. For a multi-index $|\alpha| \leq k+3$, we have for $p \in \mathbb{R}\setminus\mathbb{N}_0$

$$\partial^\alpha(u^p) = \sum_{j=1}^{|\alpha|}\left(\prod_{0\leq i\leq j-1}(p-i)\right)u^{p-j}\sum_{\substack{\alpha_1,\ldots,\alpha_j \\ \alpha_1+\ldots+\alpha_j=\alpha}}\prod_{1\leq i\leq j}\partial^{\alpha_i}u, \tag{2.70}$$

and for $p \in \mathbb{N}$

$$\partial^\alpha(u^p) = \sum_{j=1}^{\min\{|\alpha|,p\}}\left(\prod_{0\leq i\leq j-1}(p-i)\right)u^{p-j}\sum_{\substack{\alpha_1,\ldots,\alpha_j \\ \alpha_1+\ldots+\alpha_j=\alpha}}\prod_{1\leq i\leq j}\partial^{\alpha_i}u. \tag{2.71}$$

Clearly, when $p=0$, we have $\partial^\alpha(u^p) = \partial^\alpha 1 = 0$. Let $1 \leq j \leq |\alpha|$ and if $p \in \mathbb{N}_0$ also let $j \leq p$, then suppose $\alpha_1,\ldots,\alpha_j$ are multi-indices satisfying

$\alpha_1 + \cdots + \alpha_j = \alpha$. Without loss of generality, we suppose that $|\alpha_1| \geq \cdots \geq |\alpha_j|$. Let $x \in \mathbb{R}^3$ and consider the case $|\alpha_1| \leq k+2$, then using the Sobolev embedding $H^{k+4}(B_1(x)) \hookrightarrow C^{k+2,1/2}(B_1(x))$ [24, Section 5.6.3, Theorem 6], we deduce

$$
\begin{aligned}
\left\| u^{p-j} \prod_{1 \leq i \leq j} \partial^{\alpha_i} u \right\|_{L^2(B_1(x))} &\leq |B_1(x)| \|u^{p-j}\|_{L^\infty(\mathbb{R}^3)} \prod_{1 \leq i \leq j} \|\partial^{\alpha_i} u\|_{L^\infty(\mathbb{R}^3)} \\
&\leq C\widetilde{C}(p-j, M, \omega) \prod_{1 \leq i \leq j} \|u\|_{C^{k+2,1/2}(B_1(x))} \\
&\leq C\widetilde{C}(p-j, M, \omega) \|u\|^j_{H^{k+4}(B_1(x))} \\
&\leq C\widetilde{C}(p-j, M, \omega) \|m\|^j_{H^k_{\mathrm{unif}}(\mathbb{R}^3)} \\
&\leq C\widetilde{C}(p-j, M, \omega) \left(1 + \|m\|^{|\alpha|}_{H^k_{\mathrm{unif}}(\mathbb{R}^3)}\right). \qquad (2.72)
\end{aligned}
$$

Similarly, when $|\alpha_1| = k+3$, then it follows that $j = 1$ and $\alpha_1 = \alpha$, hence

$$
\begin{aligned}
\left\| u^{p-j} \prod_{1 \leq i \leq j} \partial^{\alpha_i} u \right\|_{L^2(B_1(x))} &= \left\| u^{p-1} \partial^{\alpha_1} u \right\|_{L^2(B_1(x))} \\
&\leq |B_1(x)| \|u^{p-1}\|_{L^\infty(\mathbb{R}^3)} \left\| \partial^{\alpha_1} u \right\|_{L^2(B_1(x))} \\
&\leq C\widetilde{C}(p-1, M, \omega) \|u\|_{H^{k+3}(B_1(x))} \\
&\leq C\widetilde{C}(p-1, M, \omega) \|u\|_{H^{k+4}_{\mathrm{unif}}(\mathbb{R}^3)} \\
&\leq C\widetilde{C}(p-1, M, \omega) \|m\|_{H^k_{\mathrm{unif}}(\mathbb{R}^3)}. \qquad (2.73)
\end{aligned}
$$

As the constants appearing in (2.72)–(2.73) are independent of $x \in \mathbb{R}^3$, combining (2.72)–(2.73) with either (2.70) or (2.71) gives

$$
\|u^p\|_{H^{k+3}_{\mathrm{unif}}(\mathbb{R}^3)} = \left(\sum_{|\alpha| \leq k+3} \|\partial^\alpha (u^p)\|^2_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \right)^{1/2} \leq C \left(1 + \|m\|^{k+3}_{H^k_{\mathrm{unif}}(\mathbb{R}^3)}\right), \quad (2.74)
$$

hence $u^p \in H^{k+3}_{\mathrm{unif}}(\mathbb{R}^3)$ for all $p \in \mathbb{R}$.

We now apply (2.74) to show that $\phi \in H^{k+3}_{\mathrm{unif}}(\mathbb{R}^3)$. As (u, ϕ) solve (2.2)

$$
\begin{aligned}
-\Delta u &= -\frac{5}{3} u^{7/3} + \phi u, \\
-\Delta \phi &= 4\pi (m - u^2),
\end{aligned}
$$

by (2.74) and standard elliptic regularity theory [24, Section 6.3.1, Theorem 2], for any $x \in \mathbb{R}^3$

$$\begin{aligned}
\|\phi\|_{H^{k+3}(B_1(x))} &\leq C\left(\|m-u^2\|_{H^{k+1}(B_2(x))} + \|\phi\|_{L^2(B_2(x))}\right) \\
&\leq C\left(\|m\|_{H^{k+1}(B_2(x))} + \|u^2\|_{H^{k+1}(B_2(x))} + \|\phi\|_{L^2(B_2(x))}\right) \\
&\leq C\left(\|m\|_{H^{k+1}_{\text{unif}}(\mathbb{R}^3)} + \|u^2\|_{H^{k+1}_{\text{unif}}(\mathbb{R}^3)} + \|\phi\|_{L^2_{\text{unif}}(\mathbb{R}^3)}\right) \\
&\leq C\left(1 + \|m\|_{H^{k+1}_{\text{unif}}(\mathbb{R}^3)} + \|m\|^{k+3}_{H^{k+1}_{\text{unif}}(\mathbb{R}^3)}\right) \\
&\leq C\left(1 + \|m\|^{k+3}_{H^{k+1}_{\text{unif}}(\mathbb{R}^3)}\right).
\end{aligned}$$

hence

$$\|\phi\|_{H^{k+3}_{\text{unif}}(\mathbb{R}^3)} = \sup_{x\in\mathbb{R}^3} \|\phi\|_{H^{k+3}(B_1(x))} \leq C\left(1 + \|m\|^{k+3}_{H^{k+1}_{\text{unif}}(\mathbb{R}^3)}\right). \tag{2.75}$$

We use a similar argument and apply the estimate (2.75) to deduce that $u \in H^{k+5}_{\text{unif}}(\mathbb{R}^3)$ by first establishing that $\phi u \in H^{k+3}_{\text{unif}}(\mathbb{R}^3)$. For a multi-index α satisfying $|\alpha| \leq k+3$, the Leibniz rule states

$$\partial^\alpha(\phi u) = \sum_{\beta\leq\alpha} \binom{\alpha}{\beta} \partial^{\alpha-\beta}\phi\, \partial^\beta u. \tag{2.76}$$

Let $x \in \mathbb{R}^3$ and first consider the case $\beta \leq \alpha$ and $|\beta| \leq k+2$,, then using the Sobolev embedding $H^{k+4}(B_1(x)) \hookrightarrow C^{k+2,1/2}(B_1(x))$ [24, Section 5.6.3, Theorem 6], we deduce

$$\begin{aligned}
\|\partial^{\alpha-\beta}\phi\, \partial^\beta u\|_{L^2(B_1(x))} &\leq \|\partial^{\alpha-\beta}\phi\|_{L^2(B_1(x))} \|\partial^\beta u\|_{L^\infty(\mathbb{R}^3)} \\
&\leq \|\phi\|_{H^{k+3}_{\text{unif}}(\mathbb{R}^3)} \|u\|_{C^{k+2}_{\text{unif}}(\mathbb{R}^3)} \\
&\leq C\|\phi\|_{H^{k+3}_{\text{unif}}(\mathbb{R}^3)} \|u\|_{H^{k+4}_{\text{unif}}(\mathbb{R}^3)} \\
&\leq C\left(1 + \|m\|^{k+3}_{H^{k+1}_{\text{unif}}(\mathbb{R}^3)}\right) C(k, \|m\|_{H^k_{\text{unif}}(\mathbb{R}^3)}, \omega).
\end{aligned} \tag{2.77}$$

Similarly, when $|\beta| = k+3$, then $\alpha = \beta$, so we infer

$$\begin{aligned}
\|\partial^{\alpha-\beta}\phi\, \partial^\beta u\|_{L^2(B_1(x))} = \|\partial^\beta u\|_{L^2(B_1(x))} &\leq \|u\|_{H^{k+3}_{\text{unif}}(\mathbb{R}^3)} \\
&\leq C(k, \|m\|_{H^k_{\text{unif}}(\mathbb{R}^3)}, \omega).
\end{aligned} \tag{2.78}$$

As the constants appearing in (2.77)–(2.78) are independent of $x \in \mathbb{R}^3$, combining (2.77)–(2.78) with (2.76) gives

$$\begin{aligned} \|\phi u\|_{H^{k+3}_{\mathrm{unif}}(\mathbb{R}^3)} &= \sup_{x\in\mathbb{R}^3} \|\phi u\|_{H^{k+3}(B_1(x))} \\ &\leq C\left(1+\|m\|^{k+3}_{H^{k+1}_{\mathrm{unif}}(\mathbb{R}^3)}\right) C(k, \|m\|_{H^k_{\mathrm{unif}}(\mathbb{R}^3)}, \omega). \end{aligned} \tag{2.79}$$

Using that u solves (2.2a), $-\Delta u = -\frac{5}{3}u^{7/3} + \phi u$, applying the elliptic regularity estimate [24, Section 6.3.1, Theorem 2] together with the estimates (2.74) and (2.79), we deduce that for any $x \in \mathbb{R}^3$

$$\begin{aligned} \|u\|_{H^{k+5}(B_1(x))} &\leq C\left(\|\tfrac{5}{3}u^{7/3} - \phi u\|_{H^{k+3}(B_2(x))} + \|u\|_{L^2(B_2(x))}\right) \\ &\leq C\left(\|u^{7/3}\|_{H^{k+3}(B_2(x))} + \|\phi u\|_{H^{k+3}(B_2(x))} + \|u\|_{L^2(B_2(x))}\right) \\ &\leq C\left(\|u^{7/3}\|_{H^{k+3}_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi u\|_{H^{k+3}_{\mathrm{unif}}(\mathbb{R}^3)} + \|u\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)}\right) \\ &\leq C\left(1 + \|m\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} + \|m\|^{k+3}_{H^{k+1}_{\mathrm{unif}}(\mathbb{R}^3)}\right) \\ &\qquad + C\left(1+\|m\|^{k+3}_{H^{k+1}_{\mathrm{unif}}(\mathbb{R}^3)}\right) C(k, \|m\|_{H^k_{\mathrm{unif}}(\mathbb{R}^3)}, \omega) \\ &\leq C\left(1+\|m\|^{k+3}_{H^{k+1}_{\mathrm{unif}}(\mathbb{R}^3)}\right) C(k, \|m\|_{H^k_{\mathrm{unif}}(\mathbb{R}^3)}, \omega), \end{aligned}$$

hence

$$\begin{aligned} \|u\|_{H^{k+5}_{\mathrm{unif}}(\mathbb{R}^3)} &= \sup_{x\in\mathbb{R}^3} \|u\|_{H^{k+5}(B_1(x))} \\ &\leq C\left(1+\|m\|^{k+3}_{H^{k+1}_{\mathrm{unif}}(\mathbb{R}^3)}\right) C(k, \|m\|_{H^k_{\mathrm{unif}}(\mathbb{R}^3)}, \omega). \end{aligned} \tag{2.80}$$

Combining (2.75) and (2.80) we obtain the desired estimate

$$\begin{aligned} &\|u\|_{H^{k+5}_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi\|_{H^{k+3}_{\mathrm{unif}}(\mathbb{R}^3)} \\ &\quad \leq C\left(1+\|m\|^{k+3}_{H^{k+1}_{\mathrm{unif}}(\mathbb{R}^3)}\right) C(k, \|m\|_{H^k_{\mathrm{unif}}(\mathbb{R}^3)}, \omega) =: C(k+1, \|m\|_{H^{k+1}_{\mathrm{unif}}(\mathbb{R}^3)}, \omega), \end{aligned}$$

which completes the proof of (2.69) by induction. □

2.5 Proof of Yukawa existence and uniqueness

We now show Propositions 2.4, 2.5, 2.6 and Corollary 2.7. The proofs of Propositions 2.4 and 2.5 both closely follow the proof of Proposition 2.1, though they employ different scaling arguments, which may depend on the Yukawa screening parameter. We require the following uniform regularity estimates to prove Propositions 2.4 and 2.5. The following result is essentially [16, Proposition 2.2], however as we require uniform regularity estimates in the following chapters, we provide a complete proof.

Proposition 2.12. *Let $m : \mathbb{R} \to \mathbb{R}_{\geq 0}$ satisfy*

$$\|m\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq M,$$

then for $R > 0$ define the truncated nuclear distribution $m_{R_n} = m \cdot \chi_{B_{R_n}(0)}$. There exist $R_0 = R_0(m), a_0 = a_0(m) > 0$ such that for all $R \geq R_0$ and $0 < a \leq a_0$, the unique solution to the minimisation problem

$$I_a^{\mathrm{TFW}}(m_R) = \inf \left\{ E_a^{\mathrm{TFW}}(v, m_R) \,\middle|\, \nabla v \in L^2(\mathbb{R}^3), v \in L^{10/3}(\mathbb{R}^3), v \geq 0 \right\} \tag{2.81}$$

yields the unique solution $(u_{a,R}, \phi_a)$ to

$$-\Delta u_{a,R} + \frac{5}{3} u_{a,R}^{7/3} - \phi_{a,R} u_{a,R} = 0, \tag{2.82a}$$

$$-\Delta \phi_{a,R} + a^2 \phi_{a,R} = 4\pi \left(m_R - u_{a,R}^2 \right). \tag{2.82b}$$

which satisfy the following estimates, with constant C independent of R:

$$\|u_{a,R}\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M), \tag{2.83}$$

$$\|\phi_{a,R}\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M), \tag{2.84}$$

and $u_{a,R} > 0$ on $\mathbb{R}^3$ whenever $m_R \not\equiv 0$. In particular, if $\int_{B_{R_0}(x)} m \geq c_0 > 0$ for some $x \in \mathbb{R}^3$ and $R_0, c_0 > 0$, then $a_0 = a_0(R_0, c_0) > 0$.

In the case $m \in \mathcal{M}_{L^2}(M, \omega)$, Proposition 2.12 can be extended to all $a > 0$. The following result will be used to prove Proposition 2.5.

Proposition 2.13. *Let $a_0 > 0$, $m \in \mathcal{M}_{L^2}(M,\omega)$ and for $R > 0$, define $m_R := m \cdot \chi_{B_R}$. There exists $R_0 = R_0(a_0,\omega) > 0$ such that for all*
$0 < a \leq a_0$ and $R \geq R_0$, the minimisation problem (2.81) yields the unique solution $(u_{a,R}, \phi_{a,R})$ to (2.82) which satisfy the following estimates, with constants independent of a and R:

$$\|u_{a,R}\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(a_0, M),$$
$$\|\phi_{a,R}\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(a_0, M).$$

Remark 4. The Coulomb minimisation problem Proposition 2.11 imposes a charge neutrality condition, which is essential in constructing the Coulomb ground state (u, ϕ). Imposing a neutrality condition for the finite Yukawa problem introduces a Lagrange multiplier into (2.82) that weakens Theorems 3.3 and 3.4 significantly. Due to the additional regularity of the Yukawa potential, it is not necessary to include a charge neutrality constraint in (2.81). Moreover, Proposition 2.13 will be used to construct the Yukawa ground states (u_a, ϕ_a). Later, in Theorem 4.4 from Chapter 4, we will show that $(u_a, \phi_a) \to (u, \phi)$ as $a \to \infty$ for a fixed nuclear configuration $m \in \mathcal{M}_{L^2}(M,\omega)$, hence we can recover the Coulomb ground state from the Yukawa ground states, despite not imposing charge neutrality in (2.81). □

We first prove Propositions 2.12 and 2.13, then use these results to prove Propositions 2.4 and 2.5. The proof of Proposition 2.12 largely follows the proof of Proposition 2.11; it is shown in four steps.

In Step 1, the minimisation problem (2.81) is shown to be well-posed and defines a unique solution $(u_{a,R}, \phi_{a,R})$ to (2.82), where $u_{a,R}, \phi_{a,R}$ are continuous and decay at infinity. The argument in Step 2 adapts the Solovej estimate to Yukawa systems to show: there exists $C_S > 0$ that for all $m \in \mathcal{M}_{L^2}(M,\omega)$ and $a, R > 0$

$$\tfrac{10}{9} u_{a,R}^{4/3} \leq \phi_{a,R} + C_S + a^2. \tag{2.85}$$

The aim of Step 3 is to show that there exists $a_0 = a_0(\omega), R_0 = R_0(\omega) > 0$

such that for all $0 < a \le a_0 \le 1$ and $R \ge R_0$

$$u_{a,R} > 0 \text{ on } \mathbb{R}^3.$$

Finally, in Step 4, the following estimate is established

$$\|u_{a,R}\|^{4/3}_{L^\infty(\mathbb{R}^3)} + \|\phi_{a,R}\|_{L^\infty(\mathbb{R}^3)} \le C(M) + a^2 \le C(M) + 1, \tag{2.86}$$

where the final constant is independent of a, a_0 and R. The desired estimates (2.83)-(2.84) then follow from standard elliptic regularity.

Proof of Proposition 2.12. If $m \equiv 0$, then for all $a > 0$ and $R > 0$, clearly $u_{a,R} = \phi_{a,R} = m_R = 0$ satisfies (2.82) and (2.83)–(2.84).

If $m \not\equiv 0$, then $\int_{B_{R_0}(x)} m \ge c_0 > 0$ for some $x \in \mathbb{R}^3$ and $R_0, c_0 > 0$. Without loss of generality suppose $x = 0$, otherwise translate m.

Step 1 For each $n \in \mathbb{N}$ define

$$m_R(x) = m(x) \cdot \chi_{B_R}(x),$$

and choosing $R \ge R_0$ ensures that $\int_{\mathbb{R}^3} m_R \ge c_0 > 0$, hence $m_R \not\equiv 0$. Recall

$$E_a^{\mathrm{TFW}}(v, m_R) = \int |\nabla v|^2 + \int v^{10/3} + \frac{1}{2} D_a(m_R - v^2, m_R - v^2) \ge 0.$$

For each R and $a > 0$, recall the minimisation problem (2.81)

$$I_a^{\mathrm{TFW}}(m_R) = \inf \left\{ E_a^{\mathrm{TFW}}(v, m_R) \,\middle|\, \nabla v \in L^2(\mathbb{R}^3), v \in L^{10/3}(\mathbb{R}^3), v \ge 0 \right\}.$$

By the Gagliardo–Nirenberg–Sobolev embedding [55, Theorem 2.2], $v \in L^6(\mathbb{R}^3)$ and $\|v\|_{L^6(\mathbb{R}^3)} \le C\|\nabla v\|_{L^2(\mathbb{R}^3)}$, moreover $v \in L^p(\mathbb{R}^3)$ for $p \in [10/3, 6]$. Consequently

$$\begin{aligned} 0 \le D_a(v^2, v^2) \le \|Y_a\|_{L^1(\mathbb{R}^3)} \|v\|^4_{L^4(\mathbb{R}^3)} &\le C \|v\|^{5/2}_{L^{10/3}(\mathbb{R}^3)} \|v\|^{3/2}_{L^6(\mathbb{R}^3)} \\ &\le C \|v\|^{5/2}_{L^{10/3}(\mathbb{R}^3)} \|\nabla v\|^{3/2}_{L^2(\mathbb{R}^3)}. \end{aligned}$$

Observe that there are no charge constraints on the electron density as in general $v \notin L^2(\mathbb{R}^3)$. This is chosen to ensure that no Lagrange multipliers appear in (2.82).

As $m_R \in L^{p_1}(\mathbb{R}^3), Y_a \in L^{p_2}(\mathbb{R}^3)$ for all $p_1 \in [1,2], p_2 \in [1,3)$, applying Young's inequality yields

$$\begin{aligned} D_a(m_R, v^2) &\le \|Y_a\|_{L^{5/2}(\mathbb{R}^3)} \|m_R\|_{L^1(\mathbb{R}^3)} \|v^2\|_{L^{5/3}(\mathbb{R}^3)} \le C\|v\|^2_{L^{10/3}(\mathbb{R}^3)} \\ &\le C + \frac{1}{2}\|v\|^{10/3}_{L^{10/3}(\mathbb{R}^3)}, \end{aligned}$$

it follows that

$$\begin{aligned} E_a^{\mathrm{TFW}}(v, m_R) \ge \frac{1}{2}&\left(\|\nabla v\|^2_{L^2(\mathbb{R}^3)} + \|v\|^{10/3}_{L^{10/3}(\mathbb{R}^3)} + D_a(v^2, v^2)\right) \\ &+ \frac{1}{2}D_a(m_R, m_R) - C. \end{aligned}$$

As the energy is bounded below, there exists a minimising sequence v_k satisfying

$$\|\nabla v\|^2_{L^2(\mathbb{R}^3)} + \|v\|^{10/3}_{L^{10/3}(\mathbb{R}^3)} + D_a(v^2, v^2) \le C,$$

hence there exists $u_{a,R}$ such that $\nabla u_{a,R} \in L^2(\mathbb{R}^3), u_{a,R} \in L^{10/3}(\mathbb{R}^3)$. Moreover, along a subsequence ∇v_k converges to $\nabla u_{a,R}$ weakly in $L^2(\mathbb{R}^3)$, v_k converges to $u_{a,R}$, weakly in $L^6(\mathbb{R}^3)$ and $L^{10/3}(\mathbb{R}^3)$, strongly in $L^p(B_R(0))$ for all $p \in [1,6)$ and $R > 0$ and pointwise almost everywhere. Consequently,

$$E_a^{\mathrm{TFW}}(u_{a,R}, m_R) \le \liminf_{k\to\infty} E_a^{\mathrm{TFW}}(v_k, m_R) = I_a^{\mathrm{TFW}}(m_R),$$

hence $u_{a,R}$ is a minimiser of (2.81). Define the alternate minimisation problem

$$\inf\left\{ E_a^{\mathrm{TFW}}(\sqrt{\rho}, m_R) \,\middle|\, \nabla\sqrt{\rho} \in L^2(\mathbb{R}^3), \rho \in L^{5/3}(\mathbb{R}^3), \rho \ge 0 \right\}. \tag{2.87}$$

Due to the strict convexity of $\rho \mapsto E_a^{\mathrm{TFW}}(\sqrt{\rho}, m_R)$, it follows that $\rho_{a,R} = u_{a,R}^2$ is the unique minimiser of (2.87), hence $u_{a,R}$ is the unique minimiser of (2.81).

Define

$$\phi_{a,R} = \left(m_R - u_{a,R}^2\right) * Y_a,$$

then it follows that $(u_{a,R}, \phi_{a,R})$ is the unique distributional solution to (2.82)

$$\begin{aligned}
&-\Delta u_{a,R} + \frac{5}{3} u_{a,R}^{7/3} - \phi_{a,R} u_{a,R} = 0, \\
&-\Delta \phi_{a,R} + a^2 \phi_{a,R} = 4\pi \left(m_R - u_{a,R}^2 \right).
\end{aligned}$$

Moreover, as $m_R - u_{a,R}^2 \in L^2(\mathbb{R}^3)$ and the Fourier transform of Y_a, $\widehat{Y_a}$, satisfies

$$\widehat{Y_a}(k) = \frac{1}{a^2 + |k|^2},$$

it follows that

$$\begin{aligned}
\int_{\mathbb{R}^3} |\widehat{\phi_{a,R}}(k)|^2 (a^2 + |k|^2) \, \mathrm{d}k &= \int_{\mathbb{R}^3} |\widehat{(m_R - u_{a,R}^2)}(k)|^2 |\widehat{Y_a}(k)|^2 (a^2 + |k|^2) \, \mathrm{d}k \\
&= \int_{\mathbb{R}^3} \frac{|\widehat{(m_R - u_{a,R}^2)}(k)|^2}{(a^2 + |k|^2)} \, \mathrm{d}k \\
&= \int_{\mathbb{R}^3} \left((m_R - u_{a,R}^2) * Y_a \right) \left(m_R - u_{a,R}^2 \right) \\
&= D_a(m_R - u_{a,R}^2, m_R - u_{a,R}^2).
\end{aligned}$$

It follows that $\phi_{a,R} \in H^1(\mathbb{R}^3)$ and

$$\int_{\mathbb{R}^3} |\nabla \phi_{a,R}|^2 + a^2 \int_{\mathbb{R}^3} \phi_{a,R}^2 = D_a(m_R - u_{a,R}^2, m_R - u_{a,R}^2).$$

Additionally, by applying Young's inequality yields

$$\begin{aligned}
\|\phi_{a,R}\|_{L^\infty(\mathbb{R}^3)} &\leq \|m_R\|_{L^2(\mathbb{R}^3)} \|Y_a\|_{L^2(\mathbb{R}^3)} + \leq \|u_{a,R}^2\|_{L^3(\mathbb{R}^3)} \|Y_a\|_{L^{3/2}(\mathbb{R}^3)} \\
&\leq \|m_R\|_{L^2(\mathbb{R}^3)} \|Y_a\|_{L^2(\mathbb{R}^3)} + \leq \|u_{a,R}\|_{L^6(\mathbb{R}^3)}^2 \|Y_a\|_{L^{3/2}(\mathbb{R}^3)},
\end{aligned}$$

hence by [46, Lemma II.25], $\phi_{a,R}$ is a bounded, continuous function that decays uniformly at infinity. Moreover, as $\phi_{a,R}$ solves

$$-\Delta \phi_{a,R} = -a^2 \phi_{a,R} + 4\pi (m_R - u_{a,R}^2),$$

weakly and $m_R, \phi_{a,R}, u_{a,R}^2 \in L^2_{\text{unif}}(\mathbb{R}^3)$, it follows from [24, Section 6.3.1, Theorem 1] that $\phi_{a,R} \in H^2_{\text{unif}}(\mathbb{R}^3)$. In addition, as $m_R \in L^p(\mathbb{R}^3)$ for all

$p \in [1,2]$, $Y_a \in L^1(\mathbb{R}^3)$ and $u_{a,R} \in L^{10/3}(\mathbb{R}^3)$, it follows that

$$\begin{aligned}
\|\phi_{a,R}\|_{L^{5/3}(\mathbb{R}^3)} &\leq \|m_R - u_{a,R}^2\|_{L^{5/3}}(\mathbb{R}^3)\|Y_a\|_{L^1(\mathbb{R}^3)} \\
&\leq C\left(\|m_R\|_{L^{5/3}}(\mathbb{R}^3) + \|u_{a,R}^2\|_{L^{5/3}(\mathbb{R}^3)}\right) \\
&\leq C\left(\|m_R\|_{L^{5/3}}(\mathbb{R}^3) + \|u_{a,R}\|_{L^{10/3}(\mathbb{R}^3)}^2\right).
\end{aligned}$$

To bound $u_{a,R}$ above, recall that $u_{a,R}$ solves

$$-\Delta u_{a,R} = -\frac{5}{3}u_{a,R}^{7/3} + \phi_{a,R}u_{a,R}, \tag{2.88}$$

and $u_{a,R} \in L^{10/3}(\mathbb{R}^3) \cap L^6(\mathbb{R}^3)$, $\phi_{a,R} \in L^{5/3}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$. It follows that the right-hand side of (2.88) belongs to $L^2(\mathbb{R}^3)$ and

$$\begin{aligned}
&\| - \tfrac{5}{3}u_{a,R}^{7/3} + \phi_{a,R}u_{a,R}\|_{L^2(\mathbb{R}^3)} \\
&\quad\leq \tfrac{5}{3}\|u_{a,R}^{7/3}\|_{L^2(\mathbb{R}^3)} + \|\phi_{a,R}u_{a,R}\|_{L^2(\mathbb{R}^3)} \\
&\quad\leq \tfrac{5}{3}\|u_{a,R}\|_{L^{14/3}(\mathbb{R}^3)}^{7/3} + \|\phi_{a,R}\|_{L^5(\mathbb{R}^3)}\|u_{a,R}\|_{L^{10/3}(\mathbb{R}^3)} \\
&\quad\leq \tfrac{5}{3}\|u_{a,R}\|_{L^{10/3}(\mathbb{R}^3)}^{5/6}\|u_{a,R}\|_{L^6(\mathbb{R}^3)}^{3/2} + \|\phi_{a,R}\|_{L^5(\mathbb{R}^3)}\|u_{a,R}\|_{L^{10/3}(\mathbb{R}^3)}.
\end{aligned}$$

Then for any $x \in \mathbb{R}^3$ applying the elliptic regularity estimate [24, Section 6.3.1, Theorem 1] yields

$$\begin{aligned}
\|u_{a,R}\|_{H^2(B_1(x))} &\leq C(\|\tfrac{5}{3}u_{a,R}^{7/3} - \phi_{a,R}u_{a,R}\|_{L^2(B_2(x))} + \|u_{a,R}\|_{L^2(B_2(x))}) \\
&\leq C(\|\tfrac{5}{3}u_{a,R}^{7/3} - \phi_{a,R}u_{a,R}\|_{L^2(\mathbb{R}^3)} + \|u_{a,R}\|_{L^{10/3}(B_2(x))}) \\
&\leq C(\|\tfrac{5}{3}u_{a,R}^{7/3} - \phi_{a,R}u_{a,R}\|_{L^2(\mathbb{R}^3)} + \|u_{a,R}\|_{L^{10/3}(\mathbb{R}^3)}),
\end{aligned}$$

where the constant is independent of $x \in \mathbb{R}^3$. The Sobolev embedding [24, Section 5.6.3, Theorem 6] $H^2(B_1(x)) \hookrightarrow C^{0,1/2}(B_1(x))$ implies that $u_{a,R}$ is continuous and bounded as

$$\|u_{a,R}\|_{L^\infty(B_1(x))} \leq \|u_{a,R}\|_{C^{0,1/2}(B_1(x))} \leq C\|u_{a,R}\|_{H^2(B_1(x))},$$

hence

$$\|u_{a,R}\|_{L^\infty(\mathbb{R}^3)} = \sup_{x\in\mathbb{R}^3}\|u_{a,R}\|_{L^\infty(B_1(x))} \leq \sup_{x\in\mathbb{R}^3} C\|u_{a,R}\|_{H^2(B_1(x))} < \infty.$$

It remains to show that $u_{a,R}$ decays at infinity. Recall that $u_{a,R}$ solves (2.88)

$$-\Delta u_R = -\frac{5}{3}u_R^{7/3} + \phi_R u_R$$

and also that $u_{a,R} \in L^{10/3}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3), \phi_{a,R} \in L^{5/3}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$. Define

$$g_{a,R} := \left(-\frac{5}{3}u_{a,R}^{7/3} + \phi_{a,R}u_{a,R}\right) * \tfrac{1}{|\cdot|}.$$

Observe that $u_{a,R}^{7/3} \in L^{10/7}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ and applying Hölder's inequality gives

$$\|\phi_{a,R}u_{a,R}\|_{L^{10/9}(\mathbb{R}^3)} \leq \|\phi_{a,R}\|_{L^{5/3}(\mathbb{R}^3)}\|u_{a,R}\|_{L^{10/3}(\mathbb{R}^3)},$$

hence $\phi_{a,R}u_{a,R} \in L^{10/9}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$. It then follows that $-\frac{5}{3}u_R^{7/3} + \phi_R u_R \in L^{10/7}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$. Decompose

$$\begin{aligned} g_{a,R} = &\left(-\frac{5}{3}u_{a,R}^{7/3} + \phi_{a,R}u_{a,R}\right) * \left(\tfrac{1}{|\cdot|}\chi_{B_1(0)}\right) \\ &+ \left(-\frac{5}{3}u_{a,R}^{7/3} + \phi_{a,R}u_{a,R}\right) * \left(\tfrac{1}{|\cdot|}\chi_{B_1(0)^c}\right), \end{aligned}$$

then as $\frac{1}{|\cdot|}\chi_{B_1(0)} \in L^{p_1}(\mathbb{R}^3)$ for all $p_1 \in [1,3)$, $\frac{1}{|\cdot|}\chi_{B_1^c(0)} \in L^{p_2}(\mathbb{R}^3)$ for all $p_2 \in (3,\infty]$ applying Young's inequality yields

$$\begin{aligned} \|g_{a,R}\|_{L^\infty(\mathbb{R}^3)} \leq &\|\tfrac{5}{3}u_{a,R}^{7/3} - \phi_{a,R}u_{a,R}\|_{L^2(\mathbb{R}^3)} \left\|\tfrac{1}{|\cdot|}\chi_{B_1(0)}\right\|_{L^2(\mathbb{R}^3)} \\ &+ \|\tfrac{5}{3}u_{a,R}^{7/3} - \phi_{a,R}u_{a,R}\|_{L^{10/7}(\mathbb{R}^3)} \left\|\tfrac{1}{|\cdot|}\chi_{B_1(0)^c}\right\|_{L^{10/3}(\mathbb{R}^3)}, \end{aligned}$$

hence [46, Lemma II.25] implies that $g_{a,R}$ is a continuous, bounded function vanishing at infinity. In addition, $g_{a,R}$ solves

$$-\Delta g_{a,R} = -\frac{5}{3}u_{a,R}^{7/3} + \phi_{a,R}u_{a,R} \tag{2.89}$$

in the sense of distributions. Combining (2.88) and (2.89), it follows that

$$-\Delta(u_{a,R} - g_{a,R}) = 0,$$

in the sense of distributions, so Weyl's Lemma implies that $u_{a,R} - g_{a,R}$ is harmonic [28]. Moreover, as $u_{a,R} - g_{a,R} \in L^\infty(\mathbb{R}^3)$, Liouville's Theorem implies $u_{a,R} - g_{a,R}$ is constant [28]. Suppose that $u_{a,R} - g_{a,R} = c \neq 0$, then as $g_{a,R}$ decays at infinity

$$\lim_{x\to\infty} u_{a,R}(x) = c \neq 0,$$

which contradicts $u_{a,R} \in L^{10/3}(\mathbb{R}^3)$. It follows that $u_{a,R} = g_{a,R}$ hence $u_{a,R}$ decays uniformly at infinity.

Step 2 We now adapt the argument in [62] that was used to show (2.29) in order to prove the Solovej estimate for Yukawa systems (2.85)

$$\tfrac{10}{9} u_{a,R}^{4/3} \leq \phi_{a,R} + C_S + a^2.$$

For convenience, in the following argument $u_{a,R}, \phi_{a,R}, m_{a,R}$ will be denoted as u, ϕ, m. As u solves (2.82a)

$$-\Delta u + \frac{5}{3} u^{7/3} - \phi u = 0,$$

following the proof of [62, Proposition 8], $w = u^{4/3}$ is non-negative and satisfies

$$-\Delta w + \frac{4}{3}\left(\tfrac{5}{3} w - \phi\right) w \leq 0. \tag{2.90}$$

Let $\alpha \in (0, \frac{5}{3})$ and define

$$v(x) = \alpha u^{4/3} - \phi - (C(\alpha) + a^2),$$

where $C(\alpha) = (9/4)\pi^2 \alpha^{-2} (\frac{5}{3} - \alpha)^{-1} > 0$. The expression (2.82b) can be written as

$$-\Delta \phi + a^2 \phi = 4\pi (m - w^{3/2}). \tag{2.91}$$

Combining (2.90) and (2.91), it follows that

$$\Delta v(x) \geq \frac{4\alpha}{3}\left(\tfrac{5}{3} w - \phi\right) w - 4\pi w^{3/2} + 4\pi m - a^2 \phi.$$

The aim is to prove that $v \leq 0$ by showing that $S = \{x \,|\, v(x) > 0\}$ is empty. As u, ϕ are continuous functions decaying at infinity, it follows that v is continuous, S is bounded, open and $v = 0$ on ∂S. Over S,

$$\begin{aligned}
\Delta v &\geq \frac{4\alpha}{3}\left(v + \tfrac{5}{3}w - \alpha w + (C(\alpha) + a^2)\right) w - 4\pi w^{3/2} + 4\pi m - a^2\phi \\
&\geq \frac{4\alpha}{3}\left(\tfrac{5}{3}w - \alpha w + C(\alpha) + a^2\right) w - 4\pi w^{3/2} + 4\pi m - a^2\phi \\
&= \left(\frac{4\alpha(\frac{5}{3} - \alpha)}{3}w - 4\pi w^{1/2} + \frac{4\alpha}{3}C(\alpha)\right) w + \frac{4\alpha}{3}a^2 w + 4\pi m - a^2\phi.
\end{aligned}$$

The value of $C(\alpha)$ is chosen to ensure that

$$\frac{4\alpha(\frac{5}{3} - \alpha)}{3}w - 4\pi w^{1/2} + \frac{4\alpha}{3}C(\alpha) \geq 0,$$

hence as m is non-negative and $v \geq 0$ in S

$$\begin{aligned}
\Delta v &\geq \frac{4\alpha}{3}a^2 w + 4\pi m - a^2\phi \\
&\geq a^2(\alpha w - \phi) = a^2(v + (C(\alpha) + a^2)) \geq a^2(C(\alpha) + a^2) \geq 0.
\end{aligned}$$

As v satisfies

$$\begin{aligned}
-\Delta v &\leq 0 \quad \text{in } S, \\
v &= 0 \quad \text{on } \partial S,
\end{aligned}$$

it follows that both $v \leq 0$ and $v > 0$ on S, hence S is empty and $v \leq 0$ on $\mathbb{R}^3$. So for all $\alpha \in (0, \frac{5}{3})$ and all $x \in \mathbb{R}^3$

$$\alpha u^{4/3}(x) \leq \phi(x) + C(\alpha) + a^2.$$

The right-hand side is minimised by choosing $\alpha = \frac{10}{9}$, which yields the desired estimate (2.85).

Step 3 The aim is to show that there exists $a_0 = a_0(\omega), R_0 = R_0(\omega) > 0$ such that for all $0 < a \leq a_0$ and $R \geq R_0$, $u_{a,R} > 0$ on $\mathbb{R}^3$, by following the argument used in [16, Proposition 2.2].

First recall the energy minimisation problem (2.81)

$$I_a^{\mathrm{TFW}}(m_R) = \inf \left\{ E_a^{\mathrm{TFW}}(v, m_R) \,\middle|\, \nabla v \in L^2(\mathbb{R}^3), v \in L^{10/3}(\mathbb{R}^3), v \geq 0 \right\}$$

where

$$E_a^{\mathrm{TFW}}(v, m_R) = \int_{\mathbb{R}^3} |\nabla v|^2 + \int_{\mathbb{R}^3} v^{10/3} + \frac{1}{2} D_a(m_R - v^2, m_R - v^2).$$

By showing that for large R and small $a > 0$

$$I_a^{\mathrm{TFW}}(m_R) = E_a^{\mathrm{TFW}}(u_{a,R}, m_R) < E_a^{\mathrm{TFW}}(0, m_R), \tag{2.92}$$

it follows that $u_{a,R} \geq 0$ and $u_{a,R} \not\equiv 0$. Applying the argument used in the Coulomb setting (2.38) verbatim, the Harnack inequality implies $u_{a,R} > 0$ on $\mathbb{R}^3$ [28, Theorem 8.20]. An admissible test function φ_a is constructed to satisfy: for sufficiently large R

$$I_a^{\mathrm{TFW}}(m_R) \leq E_a^{\mathrm{TFW}}(\varphi_{a_0}, m_R) < E_a^{\mathrm{TFW}}(0, m_R) = \frac{1}{2} D_a(m_R, m_R).$$

For $\varepsilon > 0$, let $\varphi_a = \varepsilon \psi_a$ and consider the difference

$$\begin{aligned} &E_a^{\mathrm{TFW}}(\varepsilon \psi_a, m_R) - E_a^{\mathrm{TFW}}(0, m_R) \\ &\qquad = \varepsilon^2 \left(\int |\nabla \psi_a|^2 - D_a(m_R, \psi_a^2) \right) + \frac{\varepsilon^4}{2} D_a(\psi_a^2, \psi_a^2) + \varepsilon^{10/3} \int \psi_a^{10/3}. \end{aligned} \tag{2.93}$$

For small $\varepsilon > 0$, the right-hand side of (2.93) is shown to be negative by first proving that there exists $a_0, C_0 > 0$ such that for all $0 < a \leq a_0$

$$\int_{\mathbb{R}^3} |\nabla \psi_a|^2 - D_a(m_R, \psi_a^2) \leq -\frac{C_0}{2} a < 0. \tag{2.94}$$

Let $\psi_0 \in C_c^\infty(B_1(0))$ satisfy $\psi_0 \geq 0$, and $\psi_0 = 1$ on $B_{1/2}(0)$, then define $\psi_a(x) = a^{3/2} \psi_0(ax)$, for $a \in (0, 1]$.

Using the definition of ψ_a gives

$$
\begin{aligned}
D_a(m_R, \psi_a^2) &= \int_{\mathbb{R}^3} (m_R * Y_a)\, \psi_a^2 \geq \frac{a^3}{4} \int_{B_{1/2a}(0)} (m_R * Y_a)\,(x)\, \mathrm{d}x \\
&= a^3 \int_{\mathbb{R}^3} \left(\int_{B_{1/2a}(0) \cap B_R(y)} m_R(x-y)\, \mathrm{d}x \right) \frac{e^{-a|y|}}{|y|}\, \mathrm{d}y \\
&= a^3 \int_{\mathbb{R}^3} \left(\int_{B_{1/2a}(-y) \cap B_R(0)} m_R(x)\, \mathrm{d}x \right) \frac{e^{-a|y|}}{|y|}\, \mathrm{d}y. \qquad (2.95)
\end{aligned}
$$

First consider for $R' > 0$

$$
\int_{B_{R'}(0)} \frac{e^{-a|y|}}{|y|}\, \mathrm{d}y = 4\pi \int_0^{R'} r e^{-ar}\, \mathrm{d}r = \frac{4\pi}{a^2} \left(1 - e^{-aR'}(1 + aR') \right),
$$

hence choosing $R' = (4a)^{-1}$ ensures that

$$
\int_{B_{1/4a}(0)} \frac{e^{-a|y|}}{|y|}\, \mathrm{d}y = \frac{4\pi}{a^2} \left(1 - \tfrac{5}{4} e^{-1/4} \right) \geq \frac{\pi}{10a^2}. \qquad (2.96)
$$

Now choose $a^* = \min\{1, (4R_0)^{-1}\}$ and suppose $R \geq R_0$, then for all $y \in B_{1/4a}(0)$, it follows from the triangle inequality that $B_{R_0}(0) \subset B_{1/2a}(-y) \cap B_R(0)$, hence

$$
\int_{B_{1/2a}(-y) \cap B_R(0)} m_R(x)\, \mathrm{d}x \geq \int_{B_{R_0}(0)} m(x)\, \mathrm{d}x \geq c_0 > 0. \qquad (2.97)
$$

Applying (2.96)–(2.97) to (2.95), it follows that for all $0 < a \leq a^*$ and $R \geq R_0$

$$
\begin{aligned}
D_a(m_R, \psi_a^2) &= \int_{\mathbb{R}^3} (m_R * Y_a)\, \psi_a^2 \\
&\geq a^3 \int_{\mathbb{R}^3} \left(\int_{B_{1/2a}(-y) \cap B_R(0)} m_R(x)\, \mathrm{d}x \right) \frac{e^{-a|y|}}{|y|}\, \mathrm{d}y \\
&= c_0 a^3 \int_{B_{1/4a}(0)} \frac{e^{-a|y|}}{|y|}\, \mathrm{d}y \geq \frac{c_0 \pi}{10} a =: C_0\, a. \qquad (2.98)
\end{aligned}
$$

Using a change of variables

$$\int_{B_{1/a}(0)} |\nabla\psi_a|^2 = a^2 \int_{B_1(0)} |\nabla\psi_0|^2 =: C_1 a^2. \tag{2.99}$$

Now define $a_0 = \min\{a^*, \frac{C_0}{2C_1}\}$, then for any $0 < a \le a_0$ and $R \ge R_0$, combining (2.98)–(2.99) yields (2.94)

$$\int |\nabla\psi_a|^2 - D_a(m_R, \psi_a^2) \le C_1 a^2 - C_0 a \le \frac{C_0}{2}\, a - C_0\, a = -\frac{C_0}{2}\, a < 0.$$

Using that $a_0, \varepsilon \in (0,1]$, the remaining terms in (2.93) can be estimated using a change of variables

$$\begin{aligned}\frac{\varepsilon^4}{2} D_a(\psi_{a_0}^2, \psi_{a_0}^2) + \varepsilon^{10/3} \int \psi_{a_0}^{10/3} &= \frac{\varepsilon^4 a_0}{2} D_0(\psi_0^2, \psi_0^2) + \varepsilon^{10/3} a_0^7 \int \psi_0^{10/3} \\ &\le \left(\frac{1}{2} D_0(\psi_0^2, \psi_0^2) + \int \psi_0^{10/3}\right) \varepsilon^4 a_0 =: C_2 \varepsilon^4 a_0. \end{aligned} \tag{2.100}$$

Applying the estimates (2.94)-(2.100) to (2.93) and choosing
$0 < \varepsilon \le \min\{1, (\frac{C_0}{3C_2})^{1/2}\}$ yields the desired result (2.92)

$$E_a^{\mathrm{TFW}}(\varepsilon\psi_a, m_R) - E_a^{\mathrm{TFW}}(0, m_R) \le \left(C_2\varepsilon^2 - \frac{C_0}{2}\right)\varepsilon^2 a_0 < 0.$$

Step 4 The aim is to show a uniform upper bound for $\phi_{a,R}$, which together with (2.85) yields the uniform estimate (2.86)

$$\|u_{a,R}\|_{L^\infty(\mathbb{R}^3)}^{4/3} + \|\phi_{a,R}\|_{L^\infty(\mathbb{R}^3)} \le C(M) + a^2 \le C(M) + 1,$$

where the constant is independent of a and R. This will be proved by adapting the argument used to show uniform regularity for finite systems with Coulomb interaction [16].

As $u_{a,R} \ge 0$, re-arranging the Solovej estimate (2.85) gives the uniform lower bound

$$\phi_{a,R} \ge -(C_S + a^2). \tag{2.101}$$

If $\phi_{a,R}$ is non-positive, then (2.86) holds as

$$\|u_{a,R}\|_{L^\infty(\mathbb{R}^3)}^{4/3} + \|\phi_{a,R}\|_{L^\infty(\mathbb{R}^3)} \leq 2(C_S + a^2) \leq 2(C_S + 1).$$

Instead, suppose that $\phi_{a,R}^+$ is non-zero at some point in $\mathbb{R}^3$. As shown in Step 1, $\phi_{a,R}$ is a continuous function that decays at infinity, hence there exists $x_{a,R} \in \mathbb{R}^3$ such that

$$\phi_{a,R}^+(x_{a,R}) = \|\phi_{a,R}^+\|_{L^\infty(\mathbb{R}^3)} > 0.$$

Without loss of generality, assume that $x_{a,R} = 0$.

In Step 1, it was shown that $u_{a,R}, \phi_{a,R} \in L^\infty(\mathbb{R}^3), \nabla u_{a,R} \in L^2(\mathbb{R}^3)$ and $\phi_{a,R} \in H^1(\mathbb{R}^3)$. Consequently, applying Lemma 2.9 implies that $L_{a,R} = -\Delta + \frac{5}{3}u_{a,R}^{4/3} - \phi_{a,R}$ is a non-negative operator.

Choose $\varphi \in C_c^\infty(B_1(0))$ satisfying $0 \leq \varphi \leq 1$, $\varphi = 1$ on $B_{1/2}(0)$, $\int_{\mathbb{R}^3} \varphi^2 = 1$ and $\int_{\mathbb{R}^3} |\nabla\varphi|^2 = c_\varphi$, then for $y \in \mathbb{R}^3$, define $\varphi_y \in C_c^\infty(B_1(y))$ by $\varphi_y = \varphi(\cdot - y)$. As $L_{a,R}$ is non-negative

$$\langle \varphi_y, L_{a,R}\varphi_y \rangle = \int_{\mathbb{R}^3} |\nabla\varphi_y|^2 + \int_{\mathbb{R}^3} \left(\frac{5}{3}u_{a,R}^{4/3} - \phi_{a,R}\right)\varphi_y^2 \geq 0,$$

which can be re-arranged and expressed using convolutions as

$$\begin{aligned}\frac{5}{3}\left(u_{a,R}^{4/3} * \varphi^2\right) &\geq \left(\phi_{a,R} * \varphi^2 - \int_{\mathbb{R}^3} |\nabla\varphi|^2\right)_+ \\ &= \left(\phi_{a,R} * \varphi^2 - c_\varphi\right)_+\end{aligned}$$

Observe that $\phi_{a,R} * \varphi^2$ solves

$$-\Delta\left(\phi_{a,R} * \varphi^2\right) + a^2\left(\phi_{a,R} * \varphi^2\right) = 4\pi\left(m_R * \varphi^2 - u_{a,R}^2 * \varphi^2\right). \tag{2.102}$$

The first term can be estimated uniformly

$$\begin{aligned}4\pi\left(m_R * \varphi^2\right)(x) &= 4\pi\int_{B_1(x)} m_R(y)\varphi^2(x-y)\,\mathrm{d}y \\ &\leq 4\pi\int_{B_1(x)} m(y)\,\mathrm{d}y \leq C_0\|m\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C_0 M.\end{aligned}$$

For the second term, observe that as $\int_{\mathbb{R}^3} \varphi^2 = 1$, one can define the probability measure for Borel sets $A \subset \mathbb{R}^3$ by $\mu(A) = \int_A \varphi^2$. Using the convexity of $t \mapsto t^{3/2}$ and applying (2.39) and Jensen's inequality with μ, we deduce

$$
\begin{aligned}
4\pi\, u_{a,R}^2 * \varphi^2(x) &\geq 4\pi u_{a,R}^2 * \varphi^2(x) \\
&= 4\pi \int_{\mathbb{R}^3} u_{a,R}^2(x-y)\varphi^2(y)\,\mathrm{d}y \\
&= 4\pi \int_{\mathbb{R}^3} \left(u_{a,R}^{4/3}(x-y)\right)^{3/2} \varphi^2(y)\,\mathrm{d}y \\
&\geq 4\pi \left(\int_{\mathbb{R}^3} u_{a,R}^{4/3}(x-y)\varphi^2(y)\,\mathrm{d}y\right)^{3/2} \\
&= 4\pi (u_{a,R}^{4/3} * \varphi^2)^{3/2} \\
&\geq 4\pi \left(\frac{3}{5}\right)^{3/2} \left(\phi_{a,R} * \varphi^2 - c_\varphi\right)_+^{3/2} \geq \left(\phi_{a,R} * \varphi^2 - c_\varphi\right)_+^{3/2}.
\end{aligned}
\tag{2.103}
$$

Combining the estimates (2.102)–(2.103) yields

$$
-\Delta\left(\phi_{a,R} * \varphi^2\right) + a^2\left(\phi_{a,R} * \varphi^2\right) + \left(\phi_{a,R} * \varphi^2 - c_\varphi\right)_+^{3/2} \leq C_0 M.
$$

Observe that as $\phi_{a,R}$ is a continuous function that decays at infinity, $\phi_{a,R} * \varphi^2$ also shares these properties. Define $f := \phi_R * \varphi^2 - c_\varphi$ and consider the set

$$
S = \{\, x \in \mathbb{R}^3 \mid f(x) > 0 \,\}.
$$

It follows that S is open and bounded and further that f satisfies

$$
\begin{aligned}
-\Delta f + a^2(f + c_\varphi) + f^{3/2} \leq C_0 M \quad &\text{on } S, \\
f = 0 \quad &\text{in } \partial S.
\end{aligned}
$$

Observe that the non-negative, constant function $g = (C_0 M)^{2/3}$ satisfies

$$
\begin{aligned}
-\Delta g + a^2(g + c_\varphi) + g^{3/2} \geq g^{3/2} = C_0 M \quad &\text{on } S, \\
f \leq g \quad &\text{in } \partial S \cup S^{\mathrm{c}}.
\end{aligned}
$$

Following the comparison principle argument (2.45) verbatim gives that

$f \leq g$, hence

$$\phi_{a,R} * \varphi^2 \leq c_\varphi + (C_0 M)^{2/3} \leq C(1 + M^{2/3}).$$

Applying (2.101), it follows that

$$\begin{aligned} \phi_{a,R}^+ * \varphi^2 = \phi_{a,R}^- * \varphi^2 + \phi_{a,R} * \varphi^2 &\leq C_S + a^2 + C(1 + M^{2/3}) \\ &= C(1 + M^{2/3}) + a^2. \end{aligned} \tag{2.104}$$

Additionally, following the argument used to show (2.47) verbatim gives

$$-\Delta \phi_{a,R}^+ \leq (-\Delta \phi_{a,R})\, \chi_{\{\phi_{a,R} > 0\}} \quad \text{in distribution.}$$

Recall (2.82b), that $-\Delta \phi_{a,R} + a^2 \phi_{a,R} = 4\pi(m_R - u_{a,R}^2)$, we then deduce that

$$\begin{aligned} -\Delta \phi_{a,R}^+ \leq -\Delta \phi_{a,R}^+ + a^2 \phi_{a,R}^+ &\leq (-\Delta \phi_{a,R} + a^2 \phi_{a,R}) \chi_{\{\phi_{a,R} > 0\}} \\ &= 4\pi \left(m_R - u_{a,R}^2\right) \chi_{\{\phi_{a,R} > 0\}} \leq 4\pi m_R \leq 4\pi m, \end{aligned} \tag{2.105}$$

in distribution.

From this point onwards, following the proof of Proposition 2.11 verbatim with the estimates (2.104)–(2.105) gives

$$\|\phi_{a,R}^+\|_{L^\infty(\mathbb{R}^3)} \leq C(1 + M) + a^2. \tag{2.106}$$

Combining (2.101)–(2.106) with the Solovej estimate (2.85), yields the desired estimate (2.86)

$$\|u_{a,R}\|_{L^\infty(\mathbb{R}^3)}^{4/3} + \|\phi_{a,R}\|_{L^\infty(\mathbb{R}^3)} \leq C(1 + M) + a^2 \leq C(1 + M).$$

Then, as in the proof of Proposition 2.11, applying elliptic regularity estimates to the system (2.82) yields the desired estimates (2.83)–(2.84).

$$\begin{aligned} \|u_{a,R}\|_{H^4_{\text{unif}}(\mathbb{R}^3)} &\leq C(M), \\ \|\phi_{a,R}\|_{H^2_{\text{unif}}(\mathbb{R}^3)} &\leq C(M). \end{aligned}$$

□

Proof of Proposition 2.13. The proof follows the steps used to show Proposition 2.12. Steps 1, 2 and 4 hold verbatim and Step 3 is modified to instead show that for any $a_0 > 0$ and $m \in \mathcal{M}_{L^2}(M, \omega)$, there exists $R_0 = R_0(a_0, \omega) > 0$ such that for any $0 < a \leq a_0$ and $R \geq R_0$, the unique minimiser $u_{a,R}$ of (2.81) satisfies

$$u_{a,R} > 0 \text{ on } \mathbb{R}^3. \tag{2.107}$$

Recall the energy minimisation problem (2.81)

$$I_a^{\mathrm{TFW}}(m_R) = \inf \left\{ E_a^{\mathrm{TFW}}(v, m_R) \,\middle|\, \nabla v \in L^2(\mathbb{R}^3), v \in L^{10/3}(\mathbb{R}^3), v \geq 0 \right\}$$

where

$$E_a^{\mathrm{TFW}}(v, m_R) = \int_{\mathbb{R}^3} |\nabla v|^2 + \int_{\mathbb{R}^3} v^{10/3} + \frac{1}{2} D_a(m_R - v^2, m_R - v^2).$$

A family of test functions φ_R is now constructed to satisfy: for large R

$$I_a^{\mathrm{TFW}}(m_R) \leq E_a^{\mathrm{TFW}}(\varphi_R, m_R) < E_a^{\mathrm{TFW}}(0, m_R) = \frac{1}{2} D_a(m_R, m_R). \tag{2.108}$$

It follows from (2.108) that

$$I_a^{\mathrm{TFW}}(m_R) = E_a^{\mathrm{TFW}}(u_{a,R}, m_R) < E_a^{\mathrm{TFW}}(0, m_R),$$

which implies that $u_{a,R} \geq 0$ and $u_{a,R} \not\equiv 0$. Applying the argument used in the Coulomb setting (2.38) verbatim, the Harnack inequality implies that $u_{a,R} > 0$ on $\mathbb{R}^3$ [28, Theorem 8.20], hence (2.107) holds.

Let $\psi_R \in C_c^\infty(B_{4R}(0))$ satisfy $\psi_R \geq 0$ and $\psi_R = 1$ on $B_{2R}(0)$. Then let $\varepsilon > 0$ and consider the difference

$$\begin{aligned} &E_a^{\mathrm{TFW}}(\varepsilon \psi_R, m_R) - E_a^{\mathrm{TFW}}(0, m_R) \\ &\qquad = \varepsilon^2 \left(\int |\nabla \psi_R|^2 - D_a(m_R, \psi_R^2) \right) + \frac{\varepsilon^4}{2} D_a(\psi_R^2, \psi_R^2) + \varepsilon^{10/3} \int \psi_R^{10/3}. \end{aligned} \tag{2.109}$$

Applying (2.12) of Lemma 2.10, there exists $R_0 > 0$ such that for any $R \geq R_0$

$$\int_{\mathbb{R}^3} |\nabla \psi_R|^2 - D_a(m_R, \psi_R^2) \leq -C_0 R^3. \tag{2.110}$$

The remaining terms in (2.109) can be estimated for $0 < \varepsilon \leq 1$, using Young's inequality for convolutions and Cauchy-Schwarz, by

$$\begin{aligned}
&\frac{\varepsilon^4}{2} D_a(\psi_R^2, \psi_R^2) + \varepsilon^4 \int \psi_R^{10/3} \\
&\quad \leq \frac{\varepsilon^4}{2} D_a(\chi_{B_{2R}(0)}, \chi_{B_{2R}(0)}) + \varepsilon^4 \int_{B_{2R}(0)} 1 \\
&\quad \leq \left(\frac{1}{2} \|Y_a\|_{L^1(\mathbb{R}^3)} \|\chi_{B_{2R}(0)}\|_{L^2(\mathbb{R}^3)}^2 + \|\chi_{B_{2R}(0)}\|_{L^1(\mathbb{R}^3)} \right) \varepsilon^4 \\
&\quad \leq C(1 + a^{-2}) R^3 \varepsilon^4 =: C_3 \varepsilon^4 R^3.
\end{aligned} \tag{2.111}$$

Combining the estimates (2.110)–(2.111) and choosing $0 < \varepsilon \leq \min\{1, (\frac{C_0}{2C_3})^{1/2}\}$ ensures that

$$E_a^{\mathrm{TFW}}(\varepsilon \psi_R, m_R) - E_a^{\mathrm{TFW}}(0, m_R) \leq \left(-C_0 + C_3 \varepsilon^2\right) \varepsilon^2 R^3 < 0,$$

hence the desired estimate (2.108) holds. □

Proof of Proposition 2.4. This follows from applying Proposition 2.12, in particular using the value of a_0 given by Proposition 2.12, then following the proof of Proposition 2.1 verbatim. □

Proof of Proposition 2.5. This holds from applying Proposition 2.13 and following the proof of Proposition 2.4 in the unbounded case verbatim. □

Next, we prove the uniqueness result Proposition 2.6 by separating the result into the two following statements.

Proposition 2.14. *There exist $a_{\mathrm{c}} = a_{\mathrm{c}}(M, \omega) > 0$ and $c_{a_{\mathrm{c}}, M, \omega} > 0$ such that for all $m \in \mathcal{M}_{L^2}(M, \omega)$ and $0 < a \leq a_{\mathrm{c}}$ the corresponding Yukawa ground state $(u_a, \phi_a) \in H^4_{\mathrm{unif}}(\mathbb{R}^3) \times H^2_{\mathrm{unif}}(\mathbb{R}^3)$ is unique and the electron density u_a satisfies*

$$\inf_{x \in \mathbb{R}^3} u_a(x) \geq c_{a_{\mathrm{c}}, M, \omega} > 0. \tag{2.112}$$

Proposition 2.15. *Let $a_0 > a_{\mathrm{c}} > 0$ and $m \in \mathcal{M}_{L^2}(M, \omega)$, then for all $0 < a \leq a_0$ the corresponding Yukawa ground state $(u_a, \phi_a) \in H^4_{\mathrm{unif}}(\mathbb{R}^3) \times H^2_{\mathrm{unif}}(\mathbb{R}^3)$ is unique and there exists $c_{a_0,M,\omega} > 0$ such that the electron density u_a satisfies*

$$\inf_{x \in \mathbb{R}^3} u_a(x) \geq c_{a_0,M,\omega} > 0. \tag{2.113}$$

Remark 5. The proof of Proposition 2.14 closely follows the proof of Proposition 2.2 and [16, Theorem 6.10], whereas proving Proposition 2.15 is considerably more involved as it requires an argument based on [16, Lemma 4.14]. Due to the nature of the argument, in particular the techniques involved, the proof of Proposition 2.15 is presented in full in Appendix A.

Proof of Proposition 2.14. The estimate (2.112) is shown by contradiction, so suppose that for any $a_{\mathrm{c}} > 0$

$$\inf_{0<a\leq a_{\mathrm{c}}} \inf_{m \in \mathcal{M}_{L^2}(M,\omega)} \inf_{x\in\mathbb{R}^3} u_a(x) = 0,$$

hence there exists sequences $a_n \downarrow 0$ satisfying $a_n \leq a_1$ for all $n \in \mathbb{N}$, $(m_n) \subset \mathcal{M}_{L^2}(M, \omega)$ and $(x_n) \subset \mathbb{R}^3$ such that for all $n \in \mathbb{N}$ the ground state (u_n, ϕ_n), corresponding to m_n with Yukawa parameter a_n, satisfies

$$u_n(x_n) \leq \frac{1}{n}.$$

Recall the uniform estimate (2.7) from Proposition 2.5

$$\|u_a\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_a\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(a_1, M),$$

It follows that

$$\left\| \tfrac{5}{3} u_n^{4/3} - \phi_n \right\|_{L^\infty(\mathbb{R}^3)} \leq \tfrac{5}{3} \|u_n\|^{4/3}_{L^\infty(\mathbb{R}^3)} + \|\phi_n\|_{L^\infty(\mathbb{R}^3)} \leq C(a_1, M), \tag{2.114}$$

where the constant is independent of $n \in \mathbb{N}$. As $\frac{5}{3} u_n^{4/3} - \phi_n \in L^\infty(\mathbb{R}^3)$, $u_n \in H^1_{\mathrm{unif}}(\mathbb{R}^3)$ and $u_n > 0$ solves

$$L_n u_n := \left(-\Delta + \frac{5}{3} u_n^{4/3} - \phi_n \right) u_n = 0,$$

applying the Harnack inequality [28, Theorem 8.20], and observing that the coefficients of L_n are uniformly estimated by (2.114), we deduce that for all $R > 0$, there exists $C = C(R, a_1, M) > 0$, independent of $n \in \mathbb{N}$, such that for all $n \in \mathbb{N}$

$$\sup_{x \in B_R(x_n)} u_n(x) \leq C \inf_{x \in B_R(x_n)} u_n(x) \leq \frac{C}{n}. \tag{2.115}$$

It follows that the sequence of functions $u_n(\cdot + x_n)$ converges uniformly to zero on compact sets. Consider the ground state (u_n, ϕ_n) corresponding to the nuclear distribution m_n.

Recall that ϕ_n satisfies

$$-\Delta\phi_n + a_n^2 \phi_n = 4\pi(m_n - u_n^2)$$

in the sense of distributions. In addition, ϕ_n and m_n satisfy

$$\|m_n(\cdot + x_n)\|_{L^2_{\text{unif}}(\mathbb{R}^3)} + \|\phi_n(\cdot + x_n)\|_{H^2_{\text{unif}}(\mathbb{R}^3)} \leq C(a_1, M).$$

It follows that along a subsequence $\phi_n(\cdot + x_n)$ converges to $\widetilde{\phi}$, weakly in $H^2(B_R(0))$, strongly in $H^1(B_R(0))$ for all $R > 0$ and pointwise almost everywhere. Applying the estimates (2.64)–(2.65) verbatim, it follows that $\widetilde{m} \in \mathcal{M}_{L^2}(M, \omega)$. As $a_n \downarrow 0$, passing to the limit of

$$-\Delta\phi_n(\cdot + x_n) + a_n^2 \phi_n(\cdot + x_n) = 4\pi \left(m_n(\cdot + x_n) - u_n^2(\cdot + x_n)\right)$$

shows that $\widetilde{\phi}$ is a distributional solution of

$$-\Delta\widetilde{\phi} = 4\pi\widetilde{m}. \tag{2.116}$$

Observe that (2.116) is identical to the equation (2.66) from the proof of Coulomb uniqueness Proposition 2.2 and recall that (2.66) leads to the contradiction $\widetilde{m} \notin \mathcal{M}_{L^2}(M, \omega)$. Applying this argument verbatim using (2.116) gives an identical contradiction, thus there exists $a_{\mathrm{c}} > 0$ and $c_{a_{\mathrm{c}}, M, \omega} > 0$ such that for all $m \in \mathcal{M}_{L^2}(M, \omega)$ and $0 < a \leq a_{\mathrm{c}}$, the corresponding Yukawa electron density u_a satisfies

$$\inf_{x \in \mathbb{R}^3} u_a(x) \geq c_{a_c,M,\omega} > 0.$$

Consequently, for $0 < a \leq a_c$, the electron density satisfies $\inf u_a > 0$, hence the arguments of [16, Chapter 6] can be applied verbatim to guarantee the uniqueness of the ground state (u_a, ϕ_a). □

Proof of Proposition 2.15. The proof of Proposition 2.15 can be found in Appendix A. □

Proof of Proposition 2.6. Combining Propositions 2.14 and 2.15 yields the desired result. □

Proof of Corollary 2.7. This is identical to the proof of Corollary 2.3, using the estimate (2.7) from Proposition 2.5 to provide the initial regularity and applying the uniform lower bound $\inf u_a \geq c_{a_0,M,\omega} > 0$ from Proposition 2.6. □

Chapter 3

Locality Estimates

The aim of this chapter is to establish locality estimates for both the TFW Coulomb and Yukawa models that characterise the response of the ground state to a perturbation of the nuclear configuration.

3.1 Outline of locality argument

We adapt the proof of uniqueness of the TFW equations in [16, 8] to obtain a pointwise stability estimate for the TFW equations. We first motivate our locality results by formally demonstrating how the arguments used to prove [16, Lemma 5.3] and [8, Theorem 2.1] can be strengthened.

To begin, we state the estimate [16, (5.33)] that appears in the proof of [16, Lemma 5.3]. Given a nuclear configuration m satisfying (H1)–(H2), suppose (u_1, ϕ_1) and (u_2, ϕ_2) both solve (2.2) and define $w = u_1 - u_2$ and $\psi = \phi_1 - \phi_2$. Also, let $\xi(x) = (1 + |x|)^{-m/2}$, for $m > 1/2$, then for $\varepsilon > 0$, define $\xi_\varepsilon(x) = \xi(\varepsilon x)$. Following the proof of [16, Lemma 5.3] up to equation (5.33) gives

$$\int_{\mathbb{R}^3} w^2\, \xi_\varepsilon^2 \leq C \int_{\mathbb{R}^3} (w^2 + \psi^2)|\nabla \xi_\varepsilon|^2, \quad \text{for all } \varepsilon > 0, \tag{3.1}$$

where $C > 0$ is independent of ε. It follows from sending $\varepsilon \to 0$ in (3.1) that $w = \psi = 0$, hence the TFW equations are unique. We remark that (3.1) also appears in the proof of [8, Theorem 2.1].

The function ξ has been chosen as it satisfies $|\nabla \xi(x)| \leq C\xi(x)$ for all

$x \in \mathbb{R}^3$ and also appears in the proof of the uniqueness result [16, Theorem 4.14]. Motivated by this choice, we introduce the specialised class of test functions

$$H^1_\gamma = \left\{ \xi \in H^1(\mathbb{R}^3) \,\middle|\, |\nabla \xi(x)| \leq \gamma |\xi(x)| \,\forall\, x \in \mathbb{R}^3 \right\} \tag{3.2}$$

for $\gamma > 0$. Observe that $e^{-\widetilde{\gamma}|\cdot - y|} \in H^1_\gamma$ for any $0 < \widetilde{\gamma} \leq \gamma$ and $y \in \mathbb{R}^3$.

To establish our locality estimate, we consider two nuclear configurations $m_1, m_2 \in \mathcal{M}_{L^2}(M, \omega)$ with corresponding ground states (u_1, ϕ_1) and (u_2, ϕ_2). Similarly, define $w = u_1 - u_2, \psi = \phi_1 - \phi_2$ and $T_m = m_1 - m_2$. Following the argument used to show (3.1) yields

$$\int_{\mathbb{R}^3} (w^2 + \psi^2)\, \xi^2 \leq C_* \bigg(\int_{\mathbb{R}^3} (w^2 + \psi^2) |\nabla \xi|^2 + \int_{\mathbb{R}^3} {T_m}^2\, \xi^2 \bigg), \tag{3.3}$$

for all $\xi \in H^1(\mathbb{R}^3)$, where $C_* > 0$. Now let $\gamma = (2C_*)^{-1/2} > 0$, then for each $\xi \in H^1_\gamma$, applying that $|\nabla \xi| \leq \gamma |\xi|$ to (3.3), we deduce

$$\int_{\mathbb{R}^3} (w^2 + \psi^2)\, \xi^2 \leq \frac{1}{2} \int_{\mathbb{R}^3} (w^2 + \psi^2) |\nabla \xi|^2 + C_* \int_{\mathbb{R}^3} {T_m}^2\, \xi^2,$$

hence

$$\int_{\mathbb{R}^3} (w^2 + \psi^2)\, \xi^2 \leq C \int_{\mathbb{R}^3} {T_m}^2\, \xi^2. \tag{3.4}$$

We generalise the estimate (3.4) to derivatives of w, ψ, then applying Sobolev estimates, we obtain by choosing $\xi(x) = e^{-\gamma|x-y|}$ for $y \in \mathbb{R}^3$

$$|w(y)|^2 + |\psi(y)|^2 \leq C \int_{\mathbb{R}^3} {T_m}^2(x)\, e^{-2\gamma|x-y|} \,\mathrm{d}x \tag{3.5}$$

for all $y \in \mathbb{R}^3$. The final estimate (3.5) characterises the local response of the electron density to a perturbation of the nuclear arrangement. Moreover, due to the uniform regularity estimates established in Chapter 2, the constants $C, \gamma > 0$ are uniform for any $m_1, m_2 \in \mathcal{M}_{L^2}(M, \omega)$.

3.2 General pointwise estimates

We now state the main results of this chapter.

3.2.1 Coulomb locality

Theorem 3.1. *Let $m_1 \in \mathcal{M}_{L^2}(M,\omega)$, and let (u_1,ϕ_1) denote the corresponding ground state. Furthermore, let $m_2 : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$ satisfy*

$$\|m_2\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq M',$$

then there exists a solution (u_2,ϕ_2) to (2.2) with $m = m_2$, satisfying $u_2 \geq 0$ and

$$\|u_2\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_2\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M'). \tag{3.6}$$

Further, there exist $C = C(M,M',\omega), \gamma = \gamma(M,M',\omega) > 0$ such that for any $\xi \in H^1_\gamma$

$$\int_{\mathbb{R}^3} \bigg(\sum_{|\alpha_1|\leq 4} |\partial^{\alpha_1}(u_1-u_2)|^2 + \sum_{|\alpha_2|\leq 2} |\partial^{\alpha_2}(\phi_1-\phi_2)|^2 \bigg)\xi^2 \leq C \int_{\mathbb{R}^3} (m_1-m_2)^2\xi^2. \tag{3.7}$$

In particular, for any $y \in \mathbb{R}^3$,

$$\sum_{|\alpha|\leq 2} |\partial^\alpha(u_1-u_2)(y)|^2 + |(\phi_1-\phi_2)(y)|^2 \leq C \int_{\mathbb{R}^3} |(m_1-m_2)(x)|^2 e^{-2\gamma|x-y|}\,\mathrm{d}x. \tag{3.8}$$

Remark 6. Since Theorem 3.2 does not assume that $m_2 \in \mathcal{M}_{L^2}(M',\omega')$, the corresponding solution (u_2,ϕ_2) is not necessarily unique. Instead, Theorem 3.1 holds for any (u_2,ϕ_2) solving (2.2), that satisfies (3.6) and $u_2 \geq 0$. □

We can generalise Theorem 3.1 to obtain higher-order pointwise estimates, but this requires *both* $\inf u_1, \inf u_2 > 0$, hence we need to assume $m_1, m_2 \in \mathcal{M}_{H^k}(M,\omega)$ for some $k \in \mathbb{N}_0$.

Theorem 3.2. *Let $k \in \mathbb{N}_0$ and $m_1, m_2 \in \mathcal{M}_{H^k}(M, \omega)$. Consider the corresponding ground states $(u_1, \phi_1), (u_2, \phi_2)$ and define*

$$w = u_1 - u_2, \quad \psi = \phi_1 - \phi_2, \quad T_m = 4\pi(m_1 - m_2).$$

Then, there exist $C = C(k, M, \omega), \gamma = \gamma(M, \omega) > 0$ such that for any $\xi \in H^1_\gamma$

$$\int_{\mathbb{R}^3} \Big(\sum_{|\alpha_1| \le k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2| \le k+2} |\partial^{\alpha_2} \psi|^2 \Big) \xi^2 \le C \int_{\mathbb{R}^3} \sum_{|\beta| \le k} |\partial^\beta T_m|^2 \xi^2. \tag{3.9}$$

In particular, for any $y \in \mathbb{R}^3$,

$$\sum_{|\alpha_1| \le k+2} |\partial^{\alpha_1} w(y)|^2 + \sum_{|\alpha_2| \le k} |\partial^{\alpha_2} \psi(y)|^2 \le C \int_{\mathbb{R}^3} \sum_{|\beta| \le k} |\partial^\beta T_m(x)|^2 e^{-2\gamma|x-y|} \, \mathrm{d}x. \tag{3.10}$$

3.2.2 Yukawa locality

The following results extend Theorems 3.1 and 3.2 to the Yukawa model.

Theorem 3.3. *Let $m_1 \in \mathcal{M}_{L^2}(M, \omega)$, and let $m_2 : \mathbb{R}^3 \to \mathbb{R}_{\ge 0}$ satisfy*

$$\|m_2\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \le M',$$

then there exists $a_1 = a_1(\omega, m_2) > 0$ such that for all $0 < a \le a_1$ there exist solutions $(u_{1,a}, \phi_{1,a})$ and $(u_{2,a}, \phi_{2,a})$ to (2.3) corresponding to m_1, m_2, where $(u_{2,a}, \phi_{2,a})$ satisfies $u_{2,a} \ge 0$ and

$$\|u_{2,a}\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_{2,a}\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \le C(M'), \tag{3.11}$$

independently of a. Define

$$w = u_{1,a} - u_{2,a}, \quad \psi = \phi_{1,a} - \phi_{2,a}, \quad T_m = 4\pi(m_1 - m_2),$$

then there exist $C = C(M, M', \omega), \gamma = \gamma(M, M', \omega) > 0$, such that for any

$\xi \in H^1_\gamma$

$$\int_{\mathbb{R}^3} \Big(\sum_{|\alpha_1| \leq 4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2| \leq 2} |\partial^{\alpha_2} \psi|^2 \Big) \xi^2 \leq C \int_{\mathbb{R}^3} T_m \xi^2. \tag{3.12}$$

In particular, for any $y \in \mathbb{R}^3$,

$$\sum_{|\alpha| \leq 2} |\partial^\alpha w(y)|^2 + |\psi(y)|^2 \leq C \int_{\mathbb{R}^3} |T_m(x)|^2 e^{-2\gamma|x-y|} \, \mathrm{d}x. \tag{3.13}$$

In order to generalise Theorem 3.3 to obtain higher-order pointwise estimates, we assume that $m_1, m_2 \in \mathcal{M}_{H^k}(M, \omega)$ for some $k \in \mathbb{N}_0$ to ensure that *both* $\inf u_1, \inf u_2 > 0$.

Theorem 3.4. *Let $a_0 > 0$, $k \in \mathbb{N}_0$, $m_1, m_2 \in \mathcal{M}_{H^k}(M, \omega)$ and for $0 < a \leq a_0$, let $(u_{1,a}, \phi_{1,a}), (u_{2,a}, \phi_{2,a})$ denote the corresponding Yukawa ground states. Define*

$$w = u_{1,a} - u_{2,a}, \quad \psi = \phi_{1,a} - \phi_{2,a}, \quad T_m = 4\pi(m_1 - m_2),$$

then there exist $C = C(a_0, k, M, \omega), \gamma = \gamma(a_0, M, \omega) > 0$, independent of a, such that for any $\xi \in H^1_\gamma$

$$\int_{\mathbb{R}^3} \Big(\sum_{|\alpha_1| \leq k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2| \leq k+2} |\partial^{\alpha_2} \psi|^2 \Big) \xi^2 \leq C \int_{\mathbb{R}^3} \sum_{|\beta| \leq k} |\partial^\beta T_m|^2 \xi^2. \tag{3.14}$$

In particular, for any $y \in \mathbb{R}^3$,

$$\sum_{|\alpha_1| \leq k+2} |\partial^{\alpha_1} w(y)|^2 + \sum_{|\alpha_2| \leq k} |\partial^{\alpha_2} \psi(y)|^2 \leq C \int_{\mathbb{R}^3} \sum_{|\beta| \leq k} |\partial^\beta T_m(x)|^2 e^{-2\gamma|x-y|} \, \mathrm{d}x.$$

3.3 Proofs of Theorems 3.1 and 3.2

To prove Theorems 3.1 and 3.2, we adapt the proof of uniqueness of the TFW equations, shown in [16, 8]. Due to the length of the argument, we shall seperate it into several intermediate results. Before proving these results, we outline the structure of the proof.

First, we state two alternative sets of assumptions on nuclear distributions m_1, m_2:

(A) Let $k = 0$, $m_1 \in \mathcal{M}_{L^2}(M, \omega)$, and let (u_1, ϕ_1) denote the corresponding ground state. Also, suppose $m_2 : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$ satisfies

$$\|m_2\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq M',$$

then by Proposition 3.1 there exists (u_2, ϕ_2) solving (2.2) corresponding to m_2, satisfying $u_2 \geq 0$ and

$$\|u_2\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_2\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M'). \tag{3.15}$$

In addition, we assume that either $m_2 \not\equiv 0$ and $u_2 > 0$, or $m_2 = u_2 = \phi_2 = 0$.

We point out that in (A) we assume $u_2 > 0$, while in Theorem 3.1 we only require $u_2 \geq 0$. The restriction $u_2 > 0$ allows us to directly use results from [16], in particular Lemma 2.9, and will be lifted via a thermodynamic limit argument in the third part of its proof on page 87.

(B) Let $k \in \mathbb{N}_0$, $m_1, m_2 \in \mathcal{M}_{H^k}(M, \omega)$ and let $(u_1, \phi_1), (u_2, \phi_2)$ denote the corresponding ground states. (Note that (B) implies (A), with $M' = C(M)$.)

Throughout the remainder of the chapter we use the notation

$$w = u_1 - u_2, \quad \psi = \phi_1 - \phi_2, \quad T_m = 4\pi(m_1 - m_2).$$

By treating the coupled system of equations as a linear system and by exploiting the coupling between the electron density and electrostatic potential arising from the Coulomb energy term of the TFW functional, we obtain the following initial estimates

Lemma 3.5. *Suppose* (A) *holds, then there exists* $C = C(M, M', \omega) > 0$ *such* *that for any* $\xi \in H^1(\mathbb{R}^3)$

$$\int_{\mathbb{R}^3} \left(w^2 + |\nabla w|^2 + |\nabla\psi|^2\right)\xi^2 \le C\left(\int_{\mathbb{R}^3} T_m\psi\xi^2 + \int_{\mathbb{R}^3}(w^2+\psi^2)|\nabla\xi|^2\right). \tag{3.16}$$

To control the ψ-dependence on the right-hand side of (3.16), we require an estimate of the form

$$\int_{\mathbb{R}^3} \psi^2\xi^2 \le C\left(\int_{\mathbb{R}^3} T_m\psi\xi^2 + \int_{\mathbb{R}^3}(w^2+\psi^2)|\nabla\xi|^2\right). \tag{3.17}$$

Suppose (3.17) holds, then applying Hölder's inequality and (3.16) yields

$$\int_{\mathbb{R}^3}(w^2+\psi^2)\xi^2 \le C'\left(\int_{\mathbb{R}^3} {T_m}^2\xi^2 + \int_{\mathbb{R}^3}(w^2+\psi^2)|\nabla\xi|^2\right).$$

To remove the term $\int(w^2+\psi^2)|\nabla\xi|^2$ on the right-hand side, we simply restrict from $\xi \in H^1$ to a narrower class of test functions,

$$H^1_\gamma = \{\, \xi \in H^1(\mathbb{R}^3) \,|\, |\nabla\xi(x)| \le \gamma|\xi(x)| \ \forall\, x \in \mathbb{R}^3 \,\},$$

where $\gamma = \min\{1, (2C')^{-1/2}\} > 0$, to show

$$\int_{\mathbb{R}^3}(w^2 + |\nabla w|^2 + \psi^2 + |\nabla\psi|^2)\xi^2 \le 2C'\int_{\mathbb{R}^3} {T_m}^2\xi^2.$$

In order to show (3.17), we apply the argument used to show [8, (2.10)]. At the same time, since the equations for (w,ψ) hold pointwise, we obtain additional estimates for $\Delta w, \Delta\psi$.

Lemma 3.6. *Suppose* (A) *holds, then there exists* $C = C(M, M', \omega), \gamma = \gamma(M, M', \omega) > 0$ *such that for any* $\xi \in H^1_\gamma$

$$\int_{\mathbb{R}^3}\left(w^2 + |\nabla w|^2 + |\Delta w|^2 + \psi^2 + |\nabla\psi|^2 + |\Delta\psi|^2\right)\xi^2 \le C\int_{\mathbb{R}^3} {T_m}^2\xi^2. \tag{3.18}$$

Clearly Lemmas 3.5 and 3.6 hold also under the assumption (B) since (B) implies (A), with $M' = C(M)$. In the case (B) where m_1, m_2 are both uniformly bounded below and have higher regularity, arguing as in Corollary 2.3

and Lemma 3.6, we obtain improved estimates for w and ψ.

Observe that in Case (B), $M' = C(M)$. Due to this, we omit the dependence of M' in the constants that appear in the following lemmas, whenever we assume (B) holds.

Lemma 3.7. *Suppose that either* (A) *or* (B) *holds, then there exist* $C = C_A(M, M', \omega), \gamma = \gamma_A(M, M', \omega) > 0$ *or* $C = C_B(k, M, \omega), \gamma = \gamma_B(M, \omega) > 0$, *where* γ_B *independent of* k, *such that for any* $\xi \in H^1_\gamma$

$$\int_{\mathbb{R}^3} \Big(\sum_{|\alpha_1| \le k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2| \le k+2} |\partial^{\alpha_2} \psi|^2 \Big) \xi^2 \le C \int_{\mathbb{R}^3} \sum_{|\beta| \le k} |\partial^\beta T_m|^2 \xi^2. \tag{3.19}$$

In particular, for any $y \in \mathbb{R}^3$,

$$\sum_{|\alpha_1| \le k+2} |\partial^{\alpha_1} w(y)|^2 + \sum_{|\alpha_2| \le k} |\partial^{\alpha_2} \psi(y)|^2 \le C \int_{\mathbb{R}^3} \sum_{|\beta| \le k} |\partial^\beta T_m(x)|^2 e^{-2\gamma|x-y|} \,\mathrm{d}x. \tag{3.20}$$

We remark that in the following proofs, all integrals are taken over $\mathbb{R}^3$, unless stated otherwise.

Proof of Lemma 3.5. Case 1. First suppose that $m_2 \not\equiv 0$ and $u_2 > 0$. Recall that $m_1 \in \mathcal{M}_{L^2}(M, \omega)$, hence by Propositions 2.1, 2.2 and (3.15)

$$\|u_1\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_1\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \le C(M),$$
$$\|u_2\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_2\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \le C(M'),$$
$$\inf_{x \in \mathbb{R}^3} u_1(x) \ge c_{M,\omega} > 0.$$

By the Sobolev embedding: for all $k \in \mathbb{N}_0$ and $x \in \mathbb{R}^3$,
$H^{k+2}(B_1(x)) \hookrightarrow C^{k,1/2}(B_1(x))$ [24, Section 5.6.3, Theorem 6], so it follows that

$$\|u_1\|_{W^{2,\infty}(\mathbb{R}^3)} + \|\phi_1\|_{L^\infty(\mathbb{R}^3)} \le C(M), \tag{3.21}$$
$$\|u_2\|_{W^{2,\infty}(\mathbb{R}^3)} + \|\phi_2\|_{L^\infty(\mathbb{R}^3)} \le C(M'), \tag{3.22}$$

hence $w = u_1 - u_2 \in H^4_{\mathrm{unif}}(\mathbb{R}^3) \cap W^{2,\infty}(\mathbb{R}^3)$, $\psi = \phi_1 - \phi_2 \in H^2_{\mathrm{unif}}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, and solve

$$-\Delta w = \frac{5}{3}\left({u_2}^{7/3} - u_1^{7/3}\right) + \phi_1 u_1 - \phi_2 u_2, \tag{3.23a}$$

$$-\Delta \psi = 4\pi\left(u_2^2 - u_1^2\right) + T_m, \tag{3.23b}$$

pointwise. Let $\xi \in H^1(\mathbb{R}^3)$ then test (3.23a) with $w\xi^2$ to obtain

$$\int \nabla w \cdot \nabla(w\xi^2) + \frac{5}{3}\int (u_1^{7/3} - u_2^{7/3}) w\xi^2 - \int (\phi_1 u_1 - \phi_2 u_2) w\xi^2 = 0. \tag{3.24}$$

We will use the following rearrangements

$$\phi_1 u_1 - \phi_2 u_2 = \frac{\phi_1 + \phi_2}{2} w + \frac{u_1 + u_2}{2}\psi,$$

$$\int \nabla w \cdot \nabla(w\xi^2) = \int |\nabla(w\xi)|^2 - \int w^2 |\nabla \xi|^2, \tag{3.25}$$

$$\int \nabla \psi \cdot \nabla(\psi\xi^2) = \int |\nabla(\psi\xi)|^2 - \int \psi^2 |\nabla \xi|^2. \tag{3.26}$$

To estimate the second term of (3.24), by Proposition 2.2 and (A), $\inf u_1 \geq c_{M,\omega} > 0$ and $u_2 > 0$. It follows that for $\nu = \frac{5}{6}\inf(u_1^{4/3} + u_2^{4/3}) \geq \frac{5}{6} c_{M,\omega}^{4/3} > 0$,

$$\begin{aligned}(u_1^{7/3} - u_2^{7/3})(u_1 - u_2) &= (u_1^{4/3} + u_2^{4/3}) w^2 + u_1 u_2 (u_1^{1/3} - u_2^{1/3}) w \\ &\geq (u_1^{4/3} + u_2^{4/3}) w^2 \\ &\geq \frac{1}{2}(u_1^{4/3} + u_2^{4/3}) w^2 + \frac{3}{5}\nu w^2. \end{aligned} \tag{3.27}$$

Combining the estimates (3.24)–(3.25) and (3.27), we obtain

$$\begin{aligned}\int |\nabla(w\xi)|^2 + \frac{5}{6}\int (u_1^{4/3} + u_2^{4/3}) w^2\xi^2 - \frac{1}{2}\int (\phi_1 + \phi_2) w^2 \xi^2 + \nu \int w^2 \xi^2 \\ \leq \int w^2 |\nabla \xi|^2 + \frac{1}{2}\int \psi (u_1^2 - u_2^2)\xi^2. \end{aligned} \tag{3.28}$$

We define the following operators

$$
\begin{aligned}
L_1 &= -\Delta + \frac{5}{3}u_1^{4/3} - \phi_1, \\
L_2 &= -\Delta + \frac{5}{3}u_2^{4/3} - \phi_2, \\
L\ &= \frac{1}{2}L_1 + \frac{1}{2}L_2 = -\Delta + \frac{5}{6}(u_1^{4/3} + u_2^{4/3}) - \frac{1}{2}(\phi_1 + \phi_2).
\end{aligned}
$$

As $u_1, u_2 > 0$, Lemma 2.9 implies that L_1, L_2 are non-negative operators, hence for any $\varphi \in H^1(\mathbb{R}^3)$

$$
\langle \varphi, L\varphi \rangle = \frac{1}{2}\langle \varphi, L_1\varphi \rangle + \frac{1}{2}\langle \varphi, L_2\varphi \rangle \geq 0. \tag{3.29}
$$

Observe that as $w \in W^{2,\infty}(\mathbb{R}^3)$ and $\xi \in H^1(\mathbb{R}^3)$, $w\xi \in H^1(\mathbb{R}^3)$. We can express (3.28) as

$$
\langle w\xi, L(w\xi) \rangle + \nu \int w^2 \xi^2 \leq \int w^2 |\nabla \xi|^2 + \frac{1}{2} \int \psi(u_1^2 - u_2^2)\xi^2. \tag{3.30}
$$

To control the final term of (3.30), we begin by testing (3.23b) with $\psi\xi^2$ to obtain

$$
\int \nabla \psi \cdot \nabla(\psi \xi^2) = 4\pi \int \psi(u_2^2 - u_1^2)\xi^2 + \int T_m \psi \xi^2. \tag{3.31}
$$

Rearranging (3.31) and applying (3.26) yields

$$
\begin{aligned}
\frac{1}{2} \int \psi(u_1^2 - u_2^2)\xi^2 &= \frac{1}{8\pi} \int T_m \psi \xi^2 - \frac{1}{8\pi} \int \nabla \psi \cdot \nabla(\psi \xi^2) \\
&= \frac{1}{8\pi} \int T_m \psi \xi^2 - \frac{1}{8\pi} \int |\nabla(\psi\xi)|^2 + \frac{1}{8\pi} \int \psi^2 |\nabla \xi|^2.
\end{aligned} \tag{3.32}
$$

Combining (3.30) and (3.32) yields

$$
\begin{aligned}
&\langle w\xi, L(w\xi) \rangle + \nu \int w^2 \xi^2 + \frac{1}{8\pi} \int |\nabla(\psi\xi)|^2 \\
&\qquad \leq \frac{1}{8\pi} \int T_m \psi \xi^2 + \int w^2 |\nabla \xi|^2 + \frac{1}{8\pi} \int \psi^2 |\nabla \xi|^2.
\end{aligned} \tag{3.33}
$$

As $\xi\nabla\psi = \nabla(\psi\xi) - \psi\nabla\xi$, we have

$$\begin{aligned}\int |\nabla\psi|^2\xi^2 &\le C\left(\int |\nabla(\psi\xi)|^2 + \int \psi^2|\nabla\xi|^2\right)\\ &\le C\left(\int T_m\psi\xi^2 + \int (w^2+\psi^2)|\nabla\xi|^2\right). \end{aligned}\tag{3.34}$$

Combining the estimates (3.33)–(3.34), we obtain

$$\begin{aligned}&\langle w\xi, L(w\xi)\rangle + \nu\int w^2\xi^2 + \int |\nabla\psi|^2\xi^2\\ &\qquad\le C\left(\int T_m\psi\xi^2 + \int (w^2+\psi^2)|\nabla\xi|^2\right). \end{aligned}\tag{3.35}$$

Next we obtain an estimate for $\int |\nabla w|^2\xi^2$, using the fact that L is a non-negative operator. We can express L as

$$L = -\Delta + f, \qquad \text{where } \; f = \frac{5(u_1^{4/3}+u_2^{4/3})}{6} - \frac{\phi_1+\phi_2}{2} \in L^\infty(\mathbb{R}^3),$$

and $\|f\|_{L^\infty(\mathbb{R}^3)} \le C(M,M')$ by (3.21)–(3.22). From (3.29), we have shown that $L = -\Delta + f \ge 0$ in the sense that $\langle \varphi, L\varphi\rangle \ge 0$ for every $\varphi \in H^1(\mathbb{R}^3)$. So for every $\varepsilon \in (0,1)$ and $\varphi \in H^1(\mathbb{R}^3)$

$$\begin{aligned}\langle \varphi, L\varphi\rangle &= (1-\varepsilon)\langle\varphi, L\varphi\rangle + \varepsilon\langle\varphi, (-\Delta+f)\varphi\rangle \ge \varepsilon\langle\varphi,(-\Delta+f)\varphi\rangle\\ &= \varepsilon\left(\int_{\mathbb{R}^3}|\nabla\varphi|^2 + \int_{\mathbb{R}^3} f\varphi^2\right) \ge \varepsilon\left(\int_{\mathbb{R}^3}|\nabla\varphi|^2 - \|f\|_{L^\infty(\mathbb{R}^3)}\int_{\mathbb{R}^3}\varphi^2\right).\end{aligned}$$

Applying this to (3.35) gives

$$\begin{aligned}&\varepsilon\int|\nabla(w\xi)|^2 + (\nu - \varepsilon\|f\|_{L^\infty(\mathbb{R}^3)})\int w^2\xi^2\\ &\qquad\le C\left(\int T_m\psi\xi^2 + \int (w^2+\psi^2)|\nabla\xi|^2\right),\end{aligned}$$

so choosing $\varepsilon = \frac{\nu}{2(\|f\|_{L^\infty}+1)}$, we deduce

$$\int |\nabla(w\xi)|^2 \le C\left(\int T_m\psi\xi^2 + \int (w^2+\psi^2)|\nabla\xi|^2\right)$$

and since $\xi\nabla w = \nabla(w\xi) - w\nabla\xi$, we deduce

$$\int |\nabla w|^2\xi^2 \leq C\left(\int T_m\psi\xi^2 + \int (w^2+\psi^2)|\nabla\xi|^2\right). \tag{3.36}$$

We combine the estimates (3.35) and (3.36) to obtain the desired estimate (3.16)

$$\int w^2\xi^2 + \int |\nabla w|^2\xi^2 + \int |\nabla\psi|^2\xi^2 \leq C\left(\int T_m\psi\xi^2 + \int (w^2+\psi^2)|\nabla\xi|^2\right)$$

and observe that this estimate is valid for any $\xi \in H^1(\mathbb{R}^3)$.

Case 2. Suppose now that $m_2 = u_2 = \phi_2 = 0$, then the argument used to show (3.28) holds to give

$$\begin{aligned}\int |\nabla(w\xi)|^2 + \frac{5}{6}\int u_1^{4/3}w^2\xi^2 - \frac{1}{2}\int \phi_1 w^2\xi^2 + \nu\int w^2\xi^2 \\ \leq \int w^2|\nabla\xi|^2 + \frac{1}{2}\int \psi u_1^2\xi^2.\end{aligned}$$

Now using that L_1 is a non-negative operator, we obtain

$$\begin{aligned}&\frac{1}{2}\int |\nabla(w\xi)|^2 + \nu\int w^2\xi^2 \\ &\leq \frac{1}{2}\langle\varphi, L_1\varphi\rangle + \frac{1}{2}\int |\nabla(w\xi)|^2 + \nu\int w^2\xi^2 \\ &= \int |\nabla(w\xi)|^2 + \frac{5}{6}\int u_1^{4/3}w^2\xi^2 - \frac{1}{2}\int \phi_1 w^2\xi^2 + \nu\int w^2\xi^2 \\ &\leq \int w^2|\nabla\xi|^2 + \frac{1}{2}\int \psi u_1^2\xi^2.\end{aligned}$$

Then applying the estimates (3.31)–(3.35) yields the desired estimate (3.16): for all $\xi \in H^1(\mathbb{R}^3)$

$$\int w^2\xi^2 + \int |\nabla w|^2\xi^2 + \int |\nabla\psi|^2\xi^2 \leq C\left(\int T_m\psi\xi^2 + \int (w^2+\psi^2)|\nabla\xi|^2\right).\square$$

Proof of Lemma 3.6. To obtain an integral estimate for ψ, first recall (3.23a), that w solves

$$-\Delta w + \frac{5}{3}\left(u_1^{7/3} - u_2^{7/3}\right) - \frac{\phi_1 + \phi_2}{2} w = \frac{u_1 + u_2}{2}\psi,$$

then testing this equation with $\psi\xi^2$, for $\xi \in H^1(\mathbb{R}^3)$, yields

$$\int \frac{u_1 + u_2}{2}\psi^2\xi^2 = -\int \Delta w \psi \xi^2 + \frac{5}{3}\int \left(u_1^{7/3} - u_2^{7/3}\right)\psi\xi^2 - \int \frac{\phi_1 + \phi_2}{2} w\psi\xi^2. \tag{3.37}$$

The first term of the right-hand side can be estimated using integration by parts

$$\begin{aligned}\left|\int \Delta w \psi \xi^2\right| &= \left|\int \nabla w \cdot \nabla\left(\psi\xi^2\right)\right| \leq \left|\int \nabla w \cdot \nabla \psi \xi^2\right| + 2\left|\int \nabla w \cdot \nabla \xi \psi \xi\right| \\ &\leq \left(\int |\nabla w|^2 \xi^2\right)^{1/2}\left(\int |\nabla \psi|^2\xi^2\right)^{1/2} + 2\left(\int |\nabla w|^2 |\nabla \xi|^2\right)^{1/2}\left(\int \psi^2\xi^2\right)^{1/2}.\end{aligned}$$

By restricting $\xi \in H^1_1$, we have $|\nabla \xi| \leq |\xi|$ hence

$$\left|\int \Delta w \psi \xi^2\right| \leq 2\left(\int |\nabla w|^2 \xi^2\right)^{1/2}\left(\int \psi^2\xi^2\right)^{1/2} + \int \left(|\nabla w|^2 + |\nabla \psi|^2\right)\xi^2. \tag{3.38}$$

By the Mean Value Theorem and (3.21)–(3.22), for each $x \in \mathbb{R}^3$, there exists $0 < c_{M,\omega} \leq \theta(x) \leq C(M)$ such that for all $x \in \mathbb{R}^3$

$$|u_1^{7/3}(x) - u_2^{7/3}| \leq \frac{7}{3}\theta(x)^{4/3}|u_1(x) - u_2(x)| \leq C(M)|w(x)|,$$

hence we can estimate the remaining terms on the right-hand side of (3.37) by

$$\begin{aligned}&\left|\frac{5}{3}\int \left(u_1^{7/3} - u_2^{7/3}\right)\psi\xi^2 - \int \frac{\phi_1 + \phi_2}{2} w\psi\xi^2\right| \\ &\qquad\qquad \leq C\int |w||\psi|\xi^2 \leq C\left(\int w^2\xi^2\right)^{1/2}\left(\int \psi^2\xi^2\right)^{1/2}. \end{aligned} \tag{3.39}$$

Combining the estimates (3.38)–(3.39) with (3.37) and using that

$\inf u_1 \geq c_{M,\omega} > 0$ and $u_2 \geq 0$, we obtain

$$\begin{aligned}\int \psi^2\xi^2 &\leq \frac{2}{c_{M,\omega}} \int \frac{u_1+u_2}{2}\psi^2\xi^2 \\ &\leq C\left[\left(\int |\nabla w|^2\xi^2\right)^{1/2} + \left(\int w^2\xi^2\right)^{1/2}\right]\left(\int \psi^2\xi^2\right)^{1/2} \\ &\quad + \int \left(|\nabla w|^2 + |\nabla \psi|^2\right)\xi^2.\end{aligned}$$

Applying Young's inequality twice and using (3.16) of Lemma 3.5 yields

$$\begin{aligned}\int \psi^2\xi^2 &\leq \frac{1}{2}\int \psi^2\xi^2 + C\int \left(w^2 + |\nabla w|^2 + |\nabla \psi|^2\right)\xi^2 \\ &\leq \frac{1}{2}\int \psi^2\xi^2 + C\left(\int T_m\psi\xi^2 + \int \left(w^2+\psi^2\right)|\nabla\xi|^2\right) \\ &\leq \frac{3}{4}\int \psi^2\xi^2 + C\left(\int {T_m}^2\xi^2 + \int \left(w^2+\psi^2\right)|\nabla\xi|^2\right),\end{aligned}$$

hence we obtain

$$\int \left(w^2 + |\nabla w|^2 + \psi^2 + |\nabla\psi|^2\right)\xi^2 \leq C_0\left(\int {T_m}^2\xi^2 + \int \left(w^2+\psi^2\right)|\nabla\xi|^2\right). \tag{3.40}$$

We further restrict the choice of the test function ξ, to remove the terms depending on w and ψ from the right-hand side. Using $C_0 = C_0(M', M, \omega) > 0$, define $\gamma = \min\{1, (2C_0)^{-1/2}\} > 0$. First note that $H^1_\gamma \subseteq H^1_1$, so for any $\xi \in H^1_\gamma$, the estimate (3.40) continues to hold. In addition, $|\nabla\xi| \leq \gamma|\xi|$, hence

$$\begin{aligned}&\int \left(w^2 + |\nabla w|^2 + \psi^2 + |\nabla\psi|^2\right)\xi^2 \leq C_0\left(\int {T_m}^2\xi^2 + \int (w^2+\psi^2)|\nabla\xi|^2\right) \\ &\leq C_0\left(\int {T_m}^2\xi^2 + \gamma^2\int (w^2+\psi^2)\xi^2\right) \leq C_0\int {T_m}^2\xi^2 + \frac{1}{2}\int (w^2+\psi^2)\xi^2.\end{aligned}$$

After re-arranging, it follows that for any $\xi \in H^1_\gamma$

$$\int \left(w^2 + |\nabla w|^2 + \psi^2 + |\nabla\psi|^2\right)\xi^2 \leq C\int {T_m}^2\xi^2.$$

Finally, as the equations (3.23) hold pointwise, squaring each equation and integrating them against ξ^2 yields

$$\int |\Delta w|^2 \xi^2 \le C \int \left(w^2 + \psi^2\right) \xi^2$$
$$\int |\Delta \psi|^2 \xi^2 \le C \int \left({T_m}^2 + w^2\right) \xi^2.$$

Combining these estimates with (3.40), we obtain the desired result (3.18)

$$\int \left(w^2 + |\nabla w|^2 + |\Delta w|^2 + \psi^2 + |\nabla \psi|^2 + |\Delta \psi|^2\right)\xi^2 \le C \int {T_m}^2 \xi^2. \qquad \square$$

Proof of Lemma 3.7. Case 1. Suppose (B) holds, so $m_i \in \mathcal{M}_{H^k}(M, \omega)$ for some $k \in \mathbb{N}_0$. By Corollary 2.3, for $i \in \{1, 2\}$

$$\|u_i\|_{H^{k+4}_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_i\|_{H^{k+2}_{\mathrm{unif}}(\mathbb{R}^3)} \le C(k, M, \omega). \tag{3.41}$$

Using integration by parts, we shall obtain integral estimates for derivatives of w in terms of derivatives of Δw. We will use the Einstein summation convention throughout this proof.

To begin, we approximate $w \in H^{k+4}_{\mathrm{unif}}(\mathbb{R}^3)$ by smooth functions $w_h \in C^\infty(\mathbb{R}^3)$ such that for all $|\beta| \le k+4$, $\partial^\beta w_h$ converges to $\partial^\beta w$ pointwise, which follows as an application of [35, Lemma A.3]. This approximation is necessary in order to obtain estimates for $\partial^\alpha w$ when $|\alpha| = k+4$.

Fix $\xi \in H^1_\gamma$ and let $|\beta| = k' \le k+2$. Then using integration by parts gives

$$\begin{aligned}
\int |\Delta\partial^\beta w_h|^2\xi^2 &= \int (\partial_{ii}\partial^\beta w_h)(\partial_{jj}\partial^\beta w_h)\xi^2\\
&= -\int (\partial_i\partial^\beta w_h)(\partial_{ijj}\partial^\beta w_h)\xi^2 - 2\int (\partial_i\partial^\beta w_h)(\partial_{jj}\partial^\beta w_h)(\partial_i\xi)\xi\\
&= \int (\partial_{ij}\partial^\beta w_h)(\partial_{ij}\partial^\beta w_h)\xi^2 + 2\int (\partial_i\partial^\beta w_h)(\partial_{ij}\partial^\beta w_h)(\partial_j\xi)\xi\\
&\qquad - 2\int (\partial_i\partial^\beta w_h)(\partial_{jj} w_h)(\partial_i\xi)\xi\\
&= \int \sum_{|\alpha|=2} |\partial^{\alpha+\beta} w|^2\xi^2 + 2\int (\partial_i\partial^\beta w_h)(\partial_{ij}\partial^\beta w_h)(\partial_j\xi)\xi\\
&\qquad - 2\int (\partial_i\partial^\beta w_h)(\partial_{jj}\partial^\beta w_h)(\partial_i\xi)\xi.
\end{aligned}$$

Summing over $|\beta| = k'$ and rearranging yields

$$\begin{aligned}
&\int \sum_{|\alpha|=k'+2} |\partial^\alpha w_h|^2\xi^2 = \int \sum_{|\beta|=k'} |\Delta\partial^\beta w_h|^2\xi^2\\
&\quad + 2\sum_{|\beta|=k'}\sum_{i,j=1}^{3}\Big(\int (\partial_i\partial^\beta w_h)(\partial_{ij}\partial^\beta w_h)(\partial_j\xi)\xi - \int (\partial_i\partial^\beta w_h)(\partial_{jj}\partial^\beta w_h)(\partial_i\xi)\xi\Big).
\end{aligned}$$

Then, using that $\xi \in H^1_\gamma \subseteq H^1_1$, hence $|\nabla\xi| \le |\xi|$, we can estimate the right-hand side using Hölder's inequality,

$$\begin{aligned}
&\int \sum_{|\alpha|=k'+2} |\partial^\alpha w_h|^2\xi^2 \le \int \sum_{|\beta|=k'} |\Delta\partial^\beta w_h|^2\xi^2\\
&+ C\sum_{|\beta|=k'}\sum_{i,j=1}^{3}\Big(\int |\partial_i\partial^\beta w_h||\partial_{ij}\partial^\beta w_h|\xi^2 + \int |\partial_i\partial^\beta w_h||\partial_{jj}\partial^\beta w_h|\xi^2\Big)\\
&\le \frac{1}{2}\int \sum_{|\alpha|=k'+2} |\partial^\alpha w_h|^2\xi^2 + C\Big(\int \sum_{|\beta_1|=k'} |\Delta\partial^{\beta_1} w_h|^2\xi^2 + \int \sum_{|\beta_2|=k'+1} |\partial^{\beta_2} w_h|^2\xi^2\Big).
\end{aligned}$$

Re-arranging this and letting $h \to 0$, we obtain

$$\sum_{|\alpha|=k'+2}\int |\partial^\alpha w|^2\xi^2 \le C\Big(\int \sum_{|\beta_1|=k'} |\partial^{\beta_1}\Delta w|^2\xi^2 + \int \sum_{|\beta_2|=k'+1} |\partial^{\beta_2} w|^2\xi^2\Big). \tag{3.42}$$

Using an identical argument, we obtain similar estimates for ψ, for $k' \le k$,

$$\sum_{|\alpha|=k'+2} \int |\partial^\alpha \psi|^2 \xi^2 \le C\Big(\int \sum_{|\beta_1|=k'} |\partial^{\beta_1} \Delta \psi|^2 \xi^2 + \int \sum_{|\beta_2|=k'+1} |\partial^{\beta_2} \psi|^2 \xi^2 \Big). \tag{3.43}$$

In the case $k' = 0$, combining (3.42), (3.43) and (3.18) yields

$$\begin{aligned} &\int \sum_{|\alpha|=2} (|\partial^\alpha w|^2 + |\partial^\alpha \psi|^2)\xi^2 \\ &\qquad \le C \int \left(|\nabla w|^2 + |\Delta w|^2 + |\nabla \psi|^2 + |\Delta \psi|^2\right) \xi^2 \le C \int {T_m}^2 \xi^2. \end{aligned}$$

We will now provide estimates for the right-hand terms of the form $\partial^\beta \Delta w, \partial^\beta \Delta \psi$. Recall (3.23)

$$\begin{aligned} -\Delta w &= \frac{5}{3}\left({u_2}^{7/3} - u_1^{7/3}\right) + \frac{\phi_1 + \phi_2}{2} w + \frac{u_1 + u_2}{2} \psi =: f_1, \\ -\Delta \psi &= 4\pi \left(u_2^2 - u_1^2\right) + T_m =: f_2. \end{aligned}$$

From (3.41) it follows that $f_1 \in H^{k+2}_{\mathrm{unif}}(\mathbb{R}^3), f_2 \in H^k_{\mathrm{unif}}(\mathbb{R}^3)$. Let $|\alpha_1| = j_1 \le k+2, |\alpha_2| = j_2 \le k$, then differentiating (3.23) yields the governing equations

$$|\partial^{\alpha_1} \Delta w| \le C(j_1, M, \omega) \sum_{|\beta_1| \le j_1} \left(|\partial^{\beta_1} w| + |\partial^{\beta_1} \psi|\right), \tag{3.44}$$

$$|\partial^{\alpha_2} \Delta \psi| \le C(j_2, M, \omega) \sum_{|\beta_2| \le j_2} \left(|\partial^{\beta_2} T_m| + |\partial^{\beta_2} w|\right). \tag{3.45}$$

Squaring (3.44)–(3.45), summing over partial derivatives and integrating against ξ^2 we deduce

$$\int \sum_{|\alpha_1|=j_1} |\partial^{\alpha_1} \Delta w|^2 \xi^2 \le C \int \sum_{|\beta_1| \le j_1} \left(|\partial^{\beta_1} w|^2 + |\partial^{\beta_1} \psi|^2\right) \xi^2, \tag{3.46}$$

$$\int \sum_{|\alpha_2|=j_2} |\partial^{\alpha_2} \Delta \psi|^2 \xi^2 \le C \int \sum_{|\beta_2| \le j_2} \left(|\partial^{\beta_2} T_m|^2 + |\partial^{\beta_2} w|^2\right) \xi^2. \tag{3.47}$$

Substituting (3.46) into (3.42) gives for $i_1 \leq k+4$

$$\begin{aligned}\int \sum_{|\alpha|=i_1} |\partial^\alpha w|^2 \xi^2 &\leq C \int \Big(\sum_{|\beta_1|=i_1-1} |\partial^{\beta_1} w|^2 + \sum_{|\beta_2|=i_1-2} |\partial^{\beta_2} \Delta w|^2 \Big) \xi^2 \\ &\leq C \int \Big(\sum_{|\beta_1|=i_1-1} |\partial^{\beta_1} w|^2 + \sum_{|\beta_1|\leq i_1-2} \left(|\partial^{\beta_1} w|^2 + |\partial^{\beta_1} \psi|^2 \right) \Big) \xi^2. \end{aligned} \tag{3.48}$$

Similarly, substituting (3.47) into (3.43) gives for $i_2 \leq k+2$

$$\begin{aligned}\int \sum_{|\alpha|=i_2} |\partial^\alpha \psi|^2 \xi^2 &\leq C \int \Big(\sum_{|\beta_1|=i_2-1} |\partial^{\beta_1} \psi|^2 + \sum_{|\beta_2|=i_2-2} |\partial^{\beta_2} \Delta \psi|^2 \Big) \xi^2 \\ &\leq C \int \Big(\sum_{|\beta_1|=i_2-1} |\partial^{\beta_1} \psi|^2 + \sum_{|\beta_2|\leq i_2-2} \left(|\partial^{\beta_2} T_m|^2 + |\partial^{\beta_2} w|^2 \right) \Big) \xi^2. \end{aligned} \tag{3.49}$$

Using (3.48) and (3.49), arguing by induction over i_1, i_2 simultaneously gives

$$\int \sum_{|\alpha|\leq k+2} \left(|\partial^\alpha w|^2 + |\partial^\alpha \psi|^2 \right) \xi^2 \leq C \int \sum_{|\beta|\leq k} |\partial^\beta T_m|^2 \xi^2.$$

To show the remaining estimate for the derivatives of w, applying (3.48) with $i_1 = k+3, k+4$ yields the estimate (3.19)

$$\int \Big(\sum_{|\alpha_1|\leq k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2|\leq k+2} |\partial^{\alpha_2} \psi|^2 \Big) \xi^2 \leq C \int \sum_{|\beta|\leq k} |\partial^\beta T_m|^2 \xi^2.$$

Now fix $y \in \mathbb{R}^3$ and choose $\xi(x) = e^{-\gamma|x-y|}$. We will now show the lower pointwise lower bound for w and ψ

$$\begin{aligned}&\sum_{|\alpha_1|\leq k+2} |\partial^{\alpha_1} w(y)|^2 + \sum_{|\alpha_2|\leq k} |\partial^{\alpha_2} \psi(y)|^2 \\ &\qquad\leq C \int \Big(\sum_{|\alpha_1|\leq k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2|\leq k+2} |\partial^{\alpha_2} \psi|^2 \Big) e^{-2\gamma|x-y|} \, \mathrm{d}x, \end{aligned} \tag{3.50}$$

where the constant C is independent of y and γ.

By Corollary 2.3, $w \in H^{k+4}(B_1(y)), \psi \in H^{k+2}(B_1(y))$, hence by the Sobolev embedding theorem [24, Section 5.6.3, Theorem 6] $w \in C^{k+2,1/2}(B_1(y))$,

$\psi \in C^{k,1/2}(B_1(y))$ and

$$\begin{aligned} \|w\|_{C^{k+2}(B_1(y))} &\le C\|w\|_{H^{k+4}(B_1(y))}, \\ \|\psi\|_{C^{k}(B_1(y))} &\le C\|\psi\|_{H^{k+2}(B_1(y))}. \end{aligned}$$

We use these estimates to show (3.50)

$$\begin{aligned} &\sum_{|\alpha_1|\le k+2} |\partial^{\alpha_1} w(y)|^2 + \sum_{|\alpha_2|\le k} |\partial^{\alpha_2}\psi(y)|^2 \\ &\qquad \le \|w\|^2_{C^{k+2,1/2}(B_1(y))} + \|\psi\|^2_{C^{k,1/2}(B_1(y))} \\ &\qquad \le C\left(\|w\|^2_{H^{k+4}(B_1(y))} + \|\psi\|^2_{H^{k+2}(B_1(y))}\right) \\ &\qquad = C\int_{B_1(y)} \left(\sum_{|\alpha_1|\le k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2|\le k+2} |\partial^{\alpha_2}\psi|^2\right) \\ &\qquad \le C\int_{\mathbb{R}^3} \left(\sum_{|\alpha_1|\le k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2|\le k+2} |\partial^{\alpha_2}\psi|^2\right) e^{-2\gamma|x-y|}\,\mathrm{d}x. \end{aligned}$$

Combining (3.19) and (3.50), we obtain the desired estimate (3.20)

$$\sum_{|\alpha_1|\le k+2} |\partial^{\alpha_1} w(y)|^2 + \sum_{|\alpha_2|\le k} |\partial^{\alpha_2}\psi(y)|^2 \le C\int \sum_{|\beta|\le k} |\partial^{\beta} T_m(x)|^2 e^{-2\gamma|x-y|}\,\mathrm{d}x.$$

Case 2. Suppose (A) holds, then as $m_1 \in \mathcal{M}_{L^2}(M,\omega)$, by Proposition 2.1 and (3.15),

$$\begin{aligned} \|u_1\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_1\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} &\le C(M), \\ \|u_2\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_2\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} &\le C(M'). \end{aligned}$$

The argument used to show (3.42) holds for $k' \le 2$, so for $\xi \in H^1_1$

$$\sum_{|\alpha_1|\le 4} \int |\partial^{\alpha_1} w|^2 \xi^2 \le C\left(\int \sum_{|\beta_1|\le 2} |\partial^{\beta_1}\Delta w|^2\xi^2 + \int \sum_{|\beta_2|\le 2} |\partial^{\beta_2} w|^2 \xi^2\right).$$

Then, as (3.46) holds with $j_1 \le 2$, applying this and (3.42) for $k' = 0$ yields

$$
\begin{aligned}
\sum_{|\alpha_1|\le 4} \int |\partial^{\alpha_1} w|^2 \xi^2 &\le C \int \sum_{|\beta_1|\le 2} \left(|\partial^{\beta_1} w|^2 + |\partial^{\beta_1}\psi|^2\right) \xi^2 \\
&\le C\bigg(\int |\Delta w|^2 \xi^2 + \int \sum_{|\beta_1|\le 1} |\partial^{\beta_1} w|^2 \xi^2 + \sum_{|\beta_2|\le 2} |\partial^{\beta_2} w|^2 \xi^2 \bigg).
\end{aligned} \tag{3.51}
$$

Similarly, the argument used to show (3.43) holds for $k' = 0$, to give

$$
\sum_{|\alpha_2|\le 2} \int |\partial^{\alpha_2}\psi|^2 \xi^2 \le C\bigg(\int |\Delta\psi|^2 \xi^2 + \int \sum_{|\beta_2|\le 1} |\partial^{\beta_2}\psi|^2 \xi^2 \bigg). \tag{3.52}
$$

Finally, combining (3.51)–(3.52) and applying (3.18) from Lemma 3.6, we obtain the desired estimate (3.19) with $k = 0$

$$
\begin{aligned}
&\sum_{|\alpha_1|\le 4} \int |\partial^{\alpha_1} w|^2 \xi^2 + \sum_{|\alpha_2|\le 2} \int |\partial^{\alpha_2}\psi|^2 \xi^2 \\
&\qquad \le C\bigg(\int \left(|\Delta w|^2 + |\Delta\psi|^2\right) \xi^2 + \int \sum_{|\beta_1|\le 1} \left(|\partial^{\beta_1} w|^2 + |\partial^{\beta_1}\psi|^2\right)\xi^2 \bigg) \\
&\qquad \le C \int {T_m}^2 \xi^2.
\end{aligned}
$$

The argument used in Case 1 holds for $k = 0$ to show the desired estimate (3.20)

$$
\sum_{|\alpha_1|\le 2} |\partial^{\alpha_1} w(y)|^2 + |\psi(y)|^2 \le C \int |T_m(x)|^2 e^{-2\gamma|x-y|}\, \mathrm{d}x. \qquad \square
$$

We have now established all technical prerequisites to prove Theorems 3.1 and 3.2.

Proof of Theorem 3.2. Applying Lemmas 3.5 – 3.7 with the assumption (B) yields the desired estimates (3.9)–(3.10). $\square$

Proof of Theorem 3.1. Case 1. Suppose $\operatorname{spt}(m_2)$ is bounded and $m_2 \not\equiv 0$. We show assumption (A) is satisfied, so by applying Lemmas 3.5 – 3.7 we obtain the desired estimates (3.7)–(3.8).

Since $m_2 \in L^2_{\mathrm{unif}}(\mathbb{R}^3)$, it follows that $m_2 \in L^1(\mathbb{R}^3)$ and since $m_2 \geq 0$ and $m_2 \not\equiv 0$, it follows that $\int m_2 > 0$. Then, define the minimisation problem

$$I^{\mathrm{TFW}}(m_2) = \inf \left\{ E^{\mathrm{TFW}}(v, m_2) \,\middle|\, v \in H^1(\mathbb{R}^3), v \geq 0, \int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m_2 > 0 \right\},$$

which yields a unique solution (u_2, ϕ_2) to (2.19), satisfying $u_2 > 0$, using [47, Theorem 7.19]. Applying Proposition 6.2, we obtain the uniform estimates

$$\|u_2\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_2\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M').$$

Case 2. Suppose $m_2 = u_2 = \phi_2 = 0$, then by definition (u_2, ϕ_2) solve (2.2) and (A) is satisfied, so Lemmas 3.5 – 3.7 imply (3.7)–(3.8).

Case 3. Suppose $\mathrm{spt}(m_2)$ is unbounded. By Proposition 2.11, there exists (u_2, ϕ_2) solving (2.2) corresponding to m_2 and satisfying $u_2 \geq 0$. As we can not guarantee that $u_2 > 0$, we can not apply Lemmas 3.5 – 3.7 directly to compare (u_1, ϕ_1) with (u_2, ϕ_2). Instead we follow the proof of Proposition 2.11 and use a thermodynamic limit argument to construct a sequence of functions $(u_{2,R_n}, \phi_{2,R_n})$ that satisfy (A) for sufficiently large R_n, which converges to (u_2, ϕ_2).

Let $R_n \uparrow \infty$ and define $m_{2,R_n} := m_2 \cdot \chi_{B_{R_n}(0)}$, then as $m_2 \in L^2_{\mathrm{unif}}(\mathbb{R}^3)$, $m_2 \geq 0$ and $m_2 \not\equiv 0$, it follows that $m_{2,R_n} \in L^1(\mathbb{R}^3)$ and for sufficiently large R_n, $\int m_{2,R_n} > 0$. By Proposition 2.11, the minimisation problem

$$I^{\mathrm{TFW}}(m_{2,R_n}) = \inf \left\{ E^{\mathrm{TFW}}(v, m_{2,R_n}) \,\middle|\, v \in H^1(\mathbb{R}^3), v \geq 0, \int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m_{2,R_n} \right\},$$

defines a unique solution $(u_{2,R_n}, \phi_{2,R_n})$ to (2.19), satisfying $u_{2,R_n} > 0$ and

$$\|u_{2,R_n}\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_{2,R_n}\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M'), \tag{3.53}$$

where the constant is independent of R_n. Passing to the limit in (3.53), there exist $u_2 \in H^4_{\mathrm{unif}}(\mathbb{R}^3), \phi_2 \in H^2_{\mathrm{unif}}(\mathbb{R}^3)$ such that, respectively, along a subsequence u_{2,R_n}, ϕ_{2,R_n} converges to u_2, ϕ_2, weakly in $H^4(B_R(0))$ and $H^2(B_R(0))$, strongly in $H^2(B_R(0))$ and $L^2(B_R(0))$ for all $R > 0$ and for all $|\alpha| \leq 2$, $\partial^\alpha u_{2,R_n}, \phi_{2,R_n}$ converges to $\partial^\alpha u_2, \phi_2$ pointwise. It follows that (u_2, ϕ_2) is a solution of (2.2) corresponding to m_2, satisfying $u_2 \geq 0$ and (3.6)

$$\|u_2\|_{H^4_{\text{unif}}(\mathbb{R}^3)} + \|\phi_2\|_{H^2_{\text{unif}}(\mathbb{R}^3)} \leq C(M').$$

In addition, $(u_1', \phi_1') = (u_1, \phi_1)$ and $(u_2', \phi_2') = (u_{2,R_n}, \phi_{2,R_n})$ satisfy assumption (A) for large R_n, so by Lemmas 3.5 – 3.7 that there exist $C, \gamma > 0$, independent of R_n, such that for large R_n and any $\xi \in H^1_\gamma$

$$\begin{aligned}\int_{\mathbb{R}^3} \Bigg(\sum_{|\alpha_1| \leq 4} |\partial^{\alpha_1}(u_1 - u_{2,R_n})|^2 + \sum_{|\alpha_2| \leq 2} |\partial^{\alpha_2}(\phi_1 - \phi_{2,R_n})|^2 \Bigg) \xi^2 \\ \leq C \int_{\mathbb{R}^3} (m_1 - m_{2,R_n})^2 \xi^2, \end{aligned} \tag{3.54}$$

and for any $y \in \mathbb{R}^3$,

$$\begin{aligned}\sum_{|\alpha_1| \leq 2} |\partial^{\alpha_1}(u_1 - u_{2,R_n})(y)|^2 + |(\phi_1 - \phi_{2,R_n})(y)|^2 \\ \leq C \int_{\mathbb{R}^3} |(m_1 - m_{2,R_n})(x)|^2 e^{-2\gamma|x-y|} \, dx. \end{aligned} \tag{3.55}$$

Using the pointwise convergence of $(u_{2,R_n}, \phi_{2,R_n})$ to (u_2, ϕ_2), applying the Dominated Convergence Theorem and sending $R_n \to \infty$ in (3.54)–(3.55) we obtain the desired estimates (3.7)–(3.8). $\square$

3.4 Proofs of Theorems 3.3 and 3.4

The proofs of Theorems 3.3 and 3.4 closely follow the proofs of Theorems 3.1 and 3.2.

First, two alternative sets of assumptions on nuclear distributions m_1, m_2 are given. In the following, (u_0, ϕ_0) denotes the corresponding Coulomb ground state solving (2.2), i.e the ground state with Yukawa parameter $a = 0$.

(A) Let $k = 0$, $m_1 \in \mathcal{M}_{L^2}(M, \omega)$, $m_2 : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$ satisfy

$$\|m_2\|_{L^2_{\text{unif}}(\mathbb{R}^3)} \leq M',$$

then by Proposition 2.4 there exist $a' = a'(\omega, m_2) > 0$ such that for all

$0 \leq a_1 \leq a_2 \leq a'$ there exists $(u_1, \phi_1) = (u_{1,a_1}, \phi_{1,a_1})$, and $(u_2, \phi_2) = (u_{2,a_2}, \phi_{2,a_2})$ solving either (2.2) or (2.3) corresponding to m_2, satisfying $\inf u_1 > 0$, $u_2 \geq 0$ and

$$\|u_2\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_2\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M').$$

In addition, assume either $m_2 \not\equiv 0$ and $u_2 > 0$ or $m_2 = u_2 = \phi_2 = 0$.

Observe that (A) assumes that $u_2 > 0$, while Theorem 3.3 only requires either $u_a \geq 0$ or $u_{2,a} \geq 0$. The restriction $u_2 > 0$ will be lifted via a thermodynamic limit argument in the third part of its proof on page 93.

(B) Let $a_0 > 0$, $k \in \mathbb{N}_0$, $m_1, m_2 \in \mathcal{M}_{H^k}(M, \omega)$, $0 \leq a_1 \leq a_2 \leq a_0$ and let $(u_1, \phi_1) = (u_{1,a_1}, \phi_{1,a_1}), (u_2, \phi_2) = (u_{2,a_2}, \phi_{2,a_2})$ denote the corresponding ground states. (Note that (B) implies (A), with $a' = a_0$ and $M' = C(a_0, M)$.)

In addition, for both (A) and (B), define

$$w = u_1 - u_2, \quad \psi = \phi_1 - \phi_2,$$

and suppose that there exists $T \in H^{k'}_{\mathrm{unif}}(\mathbb{R}^3)$, where $k' \in \{k, k+2\}$, such that (w, ψ) solves

$$-\Delta w + \frac{5}{3}\left({u_1}^{7/3} - u_2^{7/3}\right) - \phi_1 u_1 + \phi_2 u_2 = 0, \tag{3.56a}$$

$$-\Delta \psi + a_1^2 \psi = 4\pi \left(u_2^2 - u_1^2\right) + T. \tag{3.56b}$$

Lemma 3.8. *Suppose that either* (A) *or* (B) *holds, then there exist* $C = C_A(M, M', \omega)$, $\gamma = \gamma_A(M, M', \omega) > 0$ *or* $C = C_B(a_0, k', M, \omega) > 0$, $\gamma = \gamma_B(a_0, M, \omega) > 0$, *independent of both* a_1, a_2, *such that for any* $\xi \in H^1_\gamma$

$$\int_{\mathbb{R}^3} \Bigg(\sum_{|\alpha_1| \leq k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2| \leq k'+2} |\partial^{\alpha_2} \psi|^2 \Bigg) \xi^2 \leq C \int_{\mathbb{R}^3} \sum_{|\beta| \leq k'} |\partial^\beta T|^2 \xi^2. \tag{3.57}$$

In particular, for any $y \in \mathbb{R}^3$,

$$\sum_{|\alpha_1| \le k+2} |\partial^{\alpha_1} w(y)|^2 + \sum_{|\alpha_2| \le k'} |\partial^{\alpha_2} \psi(y)|^2 \le C \int_{\mathbb{R}^3} \sum_{|\beta| \le k'} |\partial^\beta T(x)|^2 e^{-2\gamma|x-y|} \, \mathrm{d}x. \tag{3.58}$$

Further, if both $a_1 = a_2 = 0$, then $C = C_B(k', M, \omega), \gamma = \gamma_B(M, \omega)$.

One of the key steps in proving Lemma 3.8 is showing

$$\int_{\mathbb{R}^3} \psi^2 \xi^2 \le C \left(\int_{\mathbb{R}^3} T \psi \xi^2 + \int_{\mathbb{R}^3} (w^2 + \psi^2) |\nabla \xi|^2 \right), \tag{3.59}$$

where the constant C is independent of a_1, a_2. However, due to the presence of the additional term in (3.56b), the argument in Lemma 3.5 directly yields

$$a_1^2 \int_{\mathbb{R}^3} \psi^2 \xi^2 \le C \left(\int_{\mathbb{R}^3} T \psi \xi^2 + \int_{\mathbb{R}^3} (w^2 + \psi^2) |\nabla \xi|^2 \right),$$

where the left-hand constant tends to 0 as $a_1 \to 0$. Instead, (3.59) is obtained by closely following the proof in the Coulomb setting.

In the following proof, all integrals are taken over $\mathbb{R}^3$.

Proof of Lemma 3.8. The argument closely follows the proof of Lemma 3.7. This proof describes the key steps of the argument.

Case 1. Suppose (B) holds, so $m_1, m_2 \in \mathcal{M}_{H^k}(M, \omega)$, so by Corollary 2.7 (or Corollary 2.3 if either $a_i = 0$) for $i \in \{1, 2\}$

$$\|u_i\|_{H^{k+4}_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_i\|_{H^{k+2}_{\mathrm{unif}}(\mathbb{R}^3)} \le C(a_0, k, M, \omega)$$

and by Proposition 2.14 $\inf u_1, \inf u_2 \ge c_{a_c, M, \omega} > 0$ (if for $i \in \{1, 2\}$ $a_i = 0$ then by Proposition 2.2 $\inf u_i \ge c_{M,\omega} > 0$). Let $\xi \in H^1(\mathbb{R}^3)$, then testing (3.56a) with $w\xi^2$ and re-arranging yields

$$\begin{aligned} \int |\nabla (w\xi)|^2 + \frac{5}{6} \int (u_1^{4/3} + u_2^{4/3}) w^2 \xi^2 - \frac{1}{2} \int (\phi_1 + \phi_2) w^2 \xi^2 + \nu \int w^2 \xi^2 \\ \le \int w^2 |\nabla \xi|^2 + \frac{1}{2} \int \psi (u_1^2 - u_2^2) \xi^2, \end{aligned} \tag{3.60}$$

where $\nu = \frac{5}{6}c_{a_c,M,\omega}^{4/3} > 0$ (or $\nu \geq \frac{5}{6}c_{M,\omega}^{4/3} > 0$ when $a_1 = a_2 = 0$). As $u_1, u_2 > 0$, Lemma 2.9 implies that

$$L = -\Delta + \tfrac{5}{6}(u_1^{4/3} + u_2^{4/3}) - \tfrac{1}{2}(\phi_1 + \phi_2)$$

is a non-negative operator, hence (3.60) can be expressed as

$$\langle w\xi, L(w\xi)\rangle + \nu \int w^2\xi^2 \leq \int w^2|\nabla\xi|^2 + \frac{1}{2}\int \psi(u_1^2 - u_2^2)\xi^2, \tag{3.61}$$

Then, testing (3.56b) with $\psi\xi^2$ and re-arranging and using $a_1 \geq 0$ gives

$$\int |\nabla(\psi\xi)|^2 \leq \int |\nabla(\psi\xi)|^2 + a_1^2\int \psi^2\xi^2 \leq \int T\psi\xi^2 + 4\pi\int \psi(u_2^2 - u_1^2)\xi^2. \tag{3.62}$$

Combining (3.61) and (3.62) and further re-arrangement yields

$$\langle w\xi, L(w\xi)\rangle + \nu\int w^2\xi^2 + \frac{1}{8\pi}\int |\nabla\psi|^2\xi^2 \leq C\left(\int T\psi\xi^2 + \int (w^2 + \psi^2)|\nabla\xi|^2\right).$$

From this point, the proof of Lemma 3.7 follows verbatim to show the estimate: there exists $C, \gamma > 0$ such that for all $\xi \in H_\gamma^1$

$$\int_{\mathbb{R}^3}\left(\sum_{|\alpha_1|\leq k+4}|\partial^{\alpha_1}w|^2 + \sum_{|\alpha_2|\leq k+2}|\partial^{\alpha_2}\psi|^2\right)\xi^2 \leq C\int_{\mathbb{R}^3}\sum_{|\beta|\leq k}|\partial^\beta T|^2\xi^2. \tag{3.63}$$

If $k' = k$, then this is the desired estimate (3.57). Alternatively, if $k' = k+2$, the remaining estimate is shown by adapting the proof of Lemma 3.7. Recall (3.56b), that ψ solves

$$-\Delta\psi = -a_1^2\psi + 4\pi\left(u_2^2 - u_1^2\right) + T \in H_{\text{unif}}^{k+2}(\mathbb{R}^3),$$

hence by standard elliptic regularity [24, Section 6.3.1, Theorem 2] $\psi \in H_{\text{unif}}^{k+4}(\mathbb{R}^3)$. It follows that

$$\int \sum_{|\alpha|\leq k+2}|\partial^\alpha\Delta\psi|^2\xi^2 \leq C(k', M, \omega)\int \sum_{|\beta|\leq k+2}\left(|\partial^\beta\psi|^2 + |\partial^\beta T|^2 + |\partial^\beta w|^2\right)\xi^2.$$

In addition, applying integration by parts, for any $k_1 \leq k+2$

$$\sum_{|\alpha|=k_1+2} \int |\partial^\alpha \psi|^2 \xi^2 \leq C\Big(\int \sum_{|\beta_1|=k_1} |\partial^{\beta_1} \Delta\psi|^2 \xi^2 + \int \sum_{|\beta_2|=k_1+1} |\partial^{\beta_2} \psi|^2 \xi^2 \Big), \tag{3.64}$$

hence combining (3.63)–(3.64) for $k_1 = k+2$ gives

$$\begin{aligned} \sum_{|\alpha|=k+4} \int |\partial^\alpha \psi|^2 \xi^2 &\leq C\Big(\int \sum_{|\beta_1|=k+2} |\partial^{\beta_1} \Delta\psi|^2 \xi^2 + \int \sum_{|\beta_2|=k+3} |\partial^{\beta_2} \psi|^2 \xi^2 \Big) \\ &\leq C\Big(\int \sum_{|\beta_1|=k+2} |\partial^{\beta_1} \Delta\psi|^2 \xi^2 + \int \sum_{|\beta_2|=k+2} |\partial^{\beta_2} \psi|^2 \xi^2 \Big) \\ &\leq C \int \sum_{|\beta|\leq k+2} \left(|\partial^\beta \psi|^2 + |\partial^\beta T|^2 + |\partial^\beta w|^2 \right) \xi^2 \\ &\leq C \int_{\mathbb{R}^3} \sum_{|\beta|\leq k+2} |\partial^\beta T|^2 \xi^2. \end{aligned} \tag{3.65}$$

Inserting (3.65) into (3.63) yields the desired estimate (3.57)

$$\int_{\mathbb{R}^3} \Big(\sum_{|\alpha_1|\leq k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2|\leq k'} |\partial^{\alpha_2} \psi|^2 \Big) \xi^2 \leq C \int_{\mathbb{R}^3} \sum_{|\beta|\leq k'} |\partial^\beta T|^2 \xi^2.$$

Let $y \in \mathbb{R}^3$, then applying (3.63) with $\xi(x) = e^{-\gamma|x-y|} \in H^1_\gamma$ and following the proof of Lemma 3.7 yields the remaining estimate (3.58).

Case 2. Suppose (A) holds, then by Proposition 2.12

$$\begin{aligned} \|u_1\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_1\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M), \\ \|u_2\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_2\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M'), \end{aligned}$$

and $\inf u_1 \geq c_{a',M,\omega} > 0$ (if $a_1 = 0$ then $\inf u_1 \geq c_{M,\omega} > 0$) and $u_2 \geq 0$. Other than this, the argument of Case 1 holds verbatim to obtain (3.57)–(3.58). □

Proof of Theorem 3.4. Let $0 < a \leq a_0$, then as $m_1, m_2 \in \mathcal{M}_{H^k}(M,\omega)$ for $k \in \mathbb{N}_0$, applying Lemma 3.8(B) with $a_1 = a_2 = a$ and
$T = 4\pi(m_1 - m_2) \in H^k_{\mathrm{unif}}(\mathbb{R}^3)$ yields the desired estimate (3.14). □

Proof of Theorem 3.3. The proof closely follows and adapts the argument used to show Theorem 3.1.

As $m_1 \in \mathcal{M}_{L^2}(M,\omega)$, by Proposition 2.5 for all $a > 0$ there exists a ground state $(u_{1,a}, \phi_{1,a})$ corresponding to m_1. It remains to show that m_2 and its corresponding solution satisfy the conditions of Lemma 3.8(A).

Case 1. Suppose $\mathrm{spt}(m_2)$ is bounded and $m_2 \not\equiv 0$. Since $m_2 \in L^2_{\mathrm{unif}}(\mathbb{R}^3)$, it follows that $m_2 \in L^1(\mathbb{R}^3)$ and since $m_2 \geq 0$ and $m_2 \not\equiv 0$, it follows that $\int m_2 > 0$. For $a > 0$, consider the minimisation problem

$$I_a^{\mathrm{TFW}}(m_2) = \inf \left\{ E_a^{\mathrm{TFW}}(v, m_2) \,\middle|\, v \in H^1(\mathbb{R}^3), v \geq 0 \right\}.$$

By Proposition 2.12, there exists $a_0 = a_0(m_2) > 0$ such that for all $0 < a \leq a_0$, the minimisation problem yields a unique solution $(u_{2,a}, \phi_{2,a})$ of (2.3), satisfying $u_{2,a} > 0$ and (3.11)

$$\|u_{2,a}\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_{2,a}\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M'),$$

independently of a. Consequently, applying Lemma 3.8(A) with $0 < a_1 = a_2 \leq a' \leq 1$ and $T = 4\pi(m_1 - m_2) \in H^k_{\mathrm{unif}}(\mathbb{R}^3)$ yields the desired estimate (3.12).

Case 2. Suppose $m_2 = u_2 = \phi_2 = 0$, then by definition (u_2, ϕ_2) solve (2.2) and (A) is satisfied, so applying Lemma 3.8(A) with $0 < a_1 = a_2 \leq a' = 1$ and $T = 4\pi(m_1 - m_2) \in H^k_{\mathrm{unif}}(\mathbb{R}^3)$ yields the desired estimate (3.12).

Case 3. Suppose $\mathrm{spt}(m_2)$ is unbounded. By Proposition 2.12, there exists $a_0 = a_0(m_2) > 0$ such that for all $0 < a \leq a_0$, there exists $(u_{2,a}, \phi_{2,a})$ solving (2.3) and satisfying $u_{2,a} \geq 0$. As it is not guaranteed that $u_{2,a} > 0$, it is not possible to apply Lemma 3.8(A) directly to compare $(u_{1,a}, \phi_{1,a})$ with $(u_{2,a}, \phi_{2,a})$. Instead, by following the proof of Proposition 2.12, a thermodynamic limit argument is used to construct a sequence of functions $(u_{2,a,R_n}, \phi_{2,a,R_n})$ which satisfy (A) for sufficiently large R_n and converge to $(u_{2,a}, \phi_{2,a})$ as $R_n \to \infty$.

Let $R_n \uparrow \infty$ and define $m_{2,R_n} := m_2 \cdot \chi_{B_{R_n}(0)}$, then as $m_2 \in L^2_{\mathrm{unif}}(\mathbb{R}^3)$, $m_2 \geq 0$ and $m_2 \not\equiv 0$, it follows that $m_{2,R_n} \in L^1(\mathbb{R}^3)$ and for sufficiently large R_n, $\int m_{2,R_n} > 0$. By Proposition 2.12, there exists $R_0 = R_0(m_2) > 0$, $a_0 = a_0(m_2) > 0$ such that for all $R_n \geq R_0$ and $0 < a \leq a_0$ the minimisation problem

$$I_a^{\mathrm{TFW}}(m_{2,R_n}) = \inf\left\{ E_a^{\mathrm{TFW}}(v, m_{2,R_n}) \,\middle|\, v \in H^1(\mathbb{R}^3), v \geq 0, \int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m_{2,R_n} \right\},$$

defines a unique solution $(u_{2,a,R_n}, \phi_{2,a,R_n})$ to (2.3), satisfying $u_{2,a,R_n} > 0$ and

$$\|u_{2,a,R_n}\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_{2,a,R_n}\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M'), \tag{3.66}$$

where the constant is independent of a, a_0 and R_n. Passing to the limit in (3.66), there exist $u_{2,a} \in H^4_{\mathrm{unif}}(\mathbb{R}^3)$, $\phi_{2,a} \in H^2_{\mathrm{unif}}(\mathbb{R}^3)$ such that, respectively, along a subsequence $u_{2,a,R_n}, \phi_{2,a,R_n}$ converges to $u_{2,a}, \phi_{2,a}$, weakly in $H^4(B_R(0))$ and $H^2(B_R(0))$, strongly in $H^2(B_R(0))$ and $L^2(B_R(0))$ for all $R > 0$ and for all $|\alpha| \leq 2$, $\partial^\alpha u_{2,a,R_n}, \phi_{2,a,R_n}$ converges to $\partial^\alpha u_{2,a}, \phi_{2,a}$ pointwise. It follows that $(u_{2,a}, \phi_{2,a})$ is a solution of (2.3) corresponding to m_2, satisfying $u_{2,a} \geq 0$ and (3.11)

$$\|u_{2,a}\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_{2,a}\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M').$$

In addition, for $0 < a \leq a' = a_0$, $(u_1', \phi_1') = (u_{1,a}, \phi_{1,a})$ and $(u_2', \phi_2') = (u_{2,a,R_n}, \phi_{2,a,R_n})$ satisfy (A) for all $R_n \geq R_0$, so by Lemma 3.8 that there exist $C, \gamma > 0$, independent of a, a_0 and R_n, such that for $R_n \geq R_0$ and any $\xi \in H^1_\gamma$

$$\begin{aligned}\int_{\mathbb{R}^3} \Bigg(\sum_{|\alpha_1| \leq 4} |\partial^{\alpha_1}(u_{1,a} - u_{2,a,R_n})|^2 + \sum_{|\alpha_2| \leq 2} |\partial^{\alpha_2}(\phi_{1,a} - \phi_{2,a,R_n})|^2 \Bigg) \xi^2 \\ \leq C \int_{\mathbb{R}^3} (m_1 - m_{2,R_n})^2 \xi^2,\end{aligned} \tag{3.67}$$

and for any $y \in \mathbb{R}^3$,

$$\begin{aligned}\sum_{|\alpha_1| \leq 2} |\partial^{\alpha_1}(u_{1,a} - u_{2,a,R_n})(y)|^2 + |(\phi_{1,a} - \phi_{2,a,R_n})(y)|^2 \\ \leq C \int_{\mathbb{R}^3} |(m_1 - m_{2,R_n})(x)|^2 e^{-2\gamma|x-y|} \, \mathrm{d}x.\end{aligned} \tag{3.68}$$

Using the pointwise convergence of $(u_{2,a,R_n}, \phi_{2,a,R_n})$ to $(u_{2,a}, \phi_{2,a})$, applying the Dominated Convergence Theorem and sending $R_n \to \infty$ in (3.67)–(3.68) gives the desired estimates (3.12)–(3.13). □

3.5 Application - locality of the charge response

The following result shows that the decay properties of the nuclear perturbation are inherited by the response of the ground state.

In the following result, other than a differing constant, the statement of the result is identical for the Coulomb and Yukawa models.

Let $k > 0$ and $m_1, m_2 \in \mathcal{M}_{L^2}(M, \omega)$.

(C) Let $(u_1, \phi_1), (u_2, \phi_2)$ denote the corresponding Coulomb ground states.

(Y) Let $a_0 > 0$ and for $0 < a \leq a_0$, let $(u_1, \phi_1) = (u_{1,a}, \phi_{1,a})$ and $(u_2, \phi_2) = (u_{2,a}, \phi_{2,a})$ denote the corresponding Yukawa ground states.

In addition, for both (C) and (Y), define

$$w = u_1 - u_2, \quad \psi = \phi_1 - \phi_2, \quad T_m = 4\pi(m_1 - m_2).$$

Corollary 3.9. *Suppose that either* (C) *or* (Y) *holds.*

1. (Exponential Decay) *If there exists $\gamma' > 0$ such that $\sum_{|\beta| \leq k} |\partial^\beta T_m(x)| \leq Ce^{-\gamma'|x|}$, then there exist $C = C_C(k, M, \omega) > 0$, $\gamma = \gamma_C(\gamma', M, \omega) > 0$ or $C = C_Y(a_0, k, M, \omega)$, $\gamma = \gamma_Y(\gamma', a_0, M, \omega) > 0$, such that*

$$\sum_{|\alpha_1| \leq k+2} |\partial^{\alpha_1} w(x)| + \sum_{|\alpha_2| \leq k} |\partial^{\alpha_2} \psi(x)| \leq Ce^{-\gamma|x|}. \tag{3.69}$$

2. (Algebraic Decay) *If there exist $C, r > 0$ such that $\sum_{|\beta| \leq k} |\partial^\beta T_m(x)| \leq C(1+|x|)^{-r}$ then there exists $C = C_C(r, k, M, \omega) > 0$ or $C = C_Y(a_0, r, k, M, \omega) > 0$ such that*

$$\sum_{|\alpha_1| \leq k+2} |\partial^{\alpha_1} w(x)| + \sum_{|\alpha_2| \leq k} |\partial^{\alpha_2} \psi(x)| \leq C(1 + |x|)^{-r}. \tag{3.70}$$

3. (Global Estimates) *If $T_m \in H^k(\mathbb{R}^3)$, then there exists $C = C_C(k, M, \omega) > 0$ or $C = C_Y(a_0, k, M, \omega) > 0$ such that*

$$\|w\|_{H^{k+4}(\mathbb{R}^3)} + \|\psi\|_{H^{k+2}(\mathbb{R}^3)} \leq C\|T_m\|_{H^k(\mathbb{R}^3)}. \tag{3.71}$$

Remark 7. The comparison results Theorems 3.1 and 3.3 require only $m_1 \in \mathcal{M}_{L^2}(M,\omega)$ but impose weaker assumptions on m_2. It is not possible to use these results to generalise Corollary 3.9 since any of the decay assumptions in (1–3) already imply that $m_2 \in \mathcal{M}_{L^2}(M,\omega')$ for some ω'.

Proof of Corollary 3.9. Suppose that (C) holds.
(1) Suppose that

$$\sum_{|\beta|\le k} |\partial^\beta T_m(y)|^2 \le C e^{-2\gamma'|y|},$$

and recall (3.10), that there exists $\widetilde{\gamma} > 0$ such that for all $x \in \mathbb{R}^3$

$$\begin{aligned}\sum_{|\alpha_1|\le k+2} |\partial^{\alpha_1} w(x)|^2 + \sum_{|\alpha_2|\le k} |\partial^{\alpha_2}\psi(x)|^2 &\le C \int_{\mathbb{R}^3} \sum_{|\beta|\le k} |\partial^\beta T_m(y)|^2 e^{-2\widetilde{\gamma}|x-y|}\, \mathrm{d}y \\ &\le C \int_{\mathbb{R}^3} e^{-2\gamma'|y|} e^{-2\widetilde{\gamma}|x-y|}\, \mathrm{d}y.\end{aligned}$$

We now show that there exists $C, \gamma > 0$ such that

$$\int_{\mathbb{R}^3} e^{-2\gamma'|y|} e^{-2\widetilde{\gamma}|x-y|}\, \mathrm{d}y \le C e^{-2\gamma|x|}. \tag{3.72}$$

First suppose $\gamma' < \widetilde{\gamma}$ and choose $\gamma = \gamma'$, then the integral becomes

$$\int_{\mathbb{R}^3} e^{-2\gamma'|y|} e^{-2\widetilde{\gamma}|x-y|}\, \mathrm{d}y = \int_{\mathbb{R}^3} e^{-2\gamma'|y|} e^{-2\gamma'|x-y|} e^{-2(\widetilde{\gamma}-\gamma')|x-y|}\, \mathrm{d}y.$$

Applying the triangle inequality gives

$$\begin{aligned}\int_{\mathbb{R}^3} e^{-2\gamma'|y|} e^{-2\widetilde{\gamma}|x-y|}\, \mathrm{d}y &\le e^{-2\gamma|x|} \int_{\mathbb{R}^3} e^{-2(\widetilde{\gamma}-\gamma')|x-y|}\, \mathrm{d}y \\ &\le \frac{C}{(\widetilde{\gamma}-\gamma')^3} e^{-2\gamma|x|}.\end{aligned}$$

In general, when $\gamma' \neq \widetilde{\gamma}$, we obtain for $\gamma = \min\{\gamma', \widetilde{\gamma}\}$

$$\int_{\mathbb{R}^3} e^{-2\gamma'|y|} e^{-2\widetilde{\gamma}|x-y|}\, \mathrm{d}y \le \frac{C}{|\widetilde{\gamma}-\gamma'|^3} e^{-2\gamma|x|}.$$

When $\gamma' = \widetilde{\gamma}$, we use that $e^{-2\widetilde{\gamma}|x|} \le e^{-\widetilde{\gamma}|x|}$ for all $x \in \mathbb{R}^3$ and simply replace

$\widetilde{\gamma}$ with $\widetilde{\gamma}/2$ in (3.72) and let $\gamma = \widetilde{\gamma}/2$ to obtain

$$\int_{\mathbb{R}^3} e^{-2\widetilde{\gamma}|y|} e^{-\widetilde{\gamma}|x-y|} \, \mathrm{d}y \leq \frac{C}{\widetilde{\gamma}^3} e^{-2\gamma|x|}.$$

In each case, this gives for some $C, \gamma > 0$ dependent on $\gamma', \widetilde{\gamma}$

$$\sum_{|\alpha_1| \leq k+2} |\partial^{\alpha_1} w(x)|^2 + \sum_{|\alpha_2| \leq k} |\partial^{\alpha_2} \psi(x)|^2 \leq C e^{-2\gamma|xs|}.$$

(2) Suppose that T_m satisfies the decay property

$$\sum_{|\beta| \leq k} |\partial^\beta m(x)| \leq C(1 + |x|)^{-r}.$$

Our aim is show that for all $y \in \mathbb{R}^3$

$$\begin{aligned} &\int_{\mathbb{R}^3} \sum_{|\beta| \leq k} |\partial^\beta T_m(x)| e^{-2\gamma|x-y|} \, \mathrm{d}x \\ &\qquad \leq C \int_{\mathbb{R}^3} (1 + |x|)^{-2r} e^{-2\gamma|x-y|} \, \mathrm{d}x \leq C(1 + |y|)^{-2r}. \end{aligned} \tag{3.73}$$

Let $R = |y|/2$, we then separate the integral over $\mathbb{R}^3$ as

$$\begin{aligned} &\int_{\mathbb{R}^3} (1 + |x|)^{-2r} e^{-2\gamma|x-y|} \, \mathrm{d}x \\ &\quad = \int_{B_R(0)} (1 + |x|)^{-2r} e^{-2\gamma|x-y|} \, \mathrm{d}x + \int_{B_R(0)^c} (1 + |x|)^{-2r} e^{-2\gamma|x-y|} \, \mathrm{d}x. \end{aligned}$$

We first estimate the integral over $B_R(0)$

$$\begin{aligned} \int_{B_R(0)} (1 + |x|)^{-2r} e^{-2\gamma|x-y|} \, \mathrm{d}x &\leq \int_{B_R(0)} e^{-2\gamma|x-y|} \, \mathrm{d}x \\ &\leq e^{-2\gamma|y|} \int_{B_R(0)} e^{2\gamma|x|} \, \mathrm{d}x \leq C R^3 e^{2\gamma R} e^{-2\gamma|y|} \\ &\leq C|y|^3 e^{\gamma|y|} e^{-2\gamma|y|} \leq C|y|^3 e^{-\gamma|y|} \\ &= C \left(|y|^3 (1 + |y|)^{2r} e^{-\gamma|y|} \right) (1 + |y|)^{-2r}. \end{aligned}$$

As the function $|y|^3(1+|y|)^{2r}e^{-\gamma|y|}$ is bounded, this gives

$$\int_{B_R(0)} (1+|x|)^{-2r} e^{-2\gamma|x-y|}\,\mathrm{d}x \leq C(1+|y|)^{-2r}. \tag{3.74}$$

We now consider the integral over $B_R(0)^c$

$$\begin{aligned}\int_{B_R(0)^c} (1+|x|)^{-2r} e^{-2\gamma|x-y|}\,\mathrm{d}x &\leq (1+|R|)^{-2r}\int_{B_R(0)^c} e^{-2\gamma|x-y|}\,\mathrm{d}x\\ &\leq \left(1+\frac{|y|}{2}\right)^{-2r}\int_{B_R(0)^c} e^{-2\gamma|x-y|}\,\mathrm{d}x\\ &\leq 4^r(1+|y|)^{-2r}\int_{\mathbb{R}^3} e^{-2\gamma|x-y|}\,\mathrm{d}x\\ &= C(1+|y|)^{-2r}. \end{aligned}\tag{3.75}$$

Combining (3.74) and (3.75) gives (3.73), then using (3.73) with (3.10) from Theorem 3.2 gives the desired estimate

$$\begin{aligned}&\sum_{|\alpha_1|\leq k+2} |\partial^{\alpha_1} w(y)|^2 + \sum_{|\alpha_2|\leq k} |\partial^{\alpha_2}\psi(y)|^2\\ &\qquad\leq \int_{\mathbb{R}^3}\sum_{|\beta|\leq k} |\partial^\beta T_m(x)| e^{-2\gamma|x-y|}\,\mathrm{d}x \leq C(1+|y|)^{-2r}.\end{aligned}$$

(3) Suppose that $T_m \in H^k(\mathbb{R}^3)$ and recall (3.9), so there exists $C, \widetilde{\gamma} > 0$ such that for all $\xi \in H_{\widetilde{\gamma}}$

$$\int_{\mathbb{R}^3}\Bigg(\sum_{|\alpha_1|\leq k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2|\leq k+2} |\partial^{\alpha_2}\psi|^2\Bigg)\xi^2 \leq C\int_{\mathbb{R}^3}\sum_{|\beta|\leq k} |\partial^\beta T_m|^2\xi^2$$

For any $0 < \gamma \leq \widetilde{\gamma}$, the test function $\xi(x) = e^{-\gamma|x|} \in H_{\widetilde{\gamma}}$. Then substituting this choice of ξ into (3.9) gives

$$\begin{aligned}&\int_{\mathbb{R}^3}\Bigg(\sum_{|\alpha_1|\leq k+4} |\partial^{\alpha_1} w(x)|^2 + \sum_{|\alpha_2|\leq k+2} |\partial^{\alpha_2}\psi(x)|^2\Bigg)e^{-2\gamma|x|}\,\mathrm{d}x\\ &\qquad\qquad\leq C\int_{\mathbb{R}^3}\sum_{|\beta|\leq k} |\partial^\beta T_m(x)|^2 e^{-2\gamma|x|}\,\mathrm{d}x.\end{aligned}$$

As $T_m \in H^k(\mathbb{R}^3)$, we can simply send γ to 0 to obtain the desired estimate

$$\begin{aligned}
\|w\|^2_{H^{k+4}(\mathbb{R}^3)} + \|\psi\|^2_{H^{k+2}(\mathbb{R}^3)} &= \int_{\mathbb{R}^3} \left(\sum_{|\alpha_1| \le k+4} |\partial^{\alpha_1} w|^2 + \sum_{|\alpha_2| \le k+2} |\partial^{\alpha_2} \psi|^2 \right) \\
&\le C \int_{\mathbb{R}^3} \sum_{|\beta| \le k} |\partial^{\beta} T_m|^2 = C\|T_m\|^2_{H^k(\mathbb{R}^3)}.
\end{aligned}$$

Suppose (Y) holds, other than applying Theorem 3.4 instead of Theorem 3.2, the proofs of (1–3) follow from the case (C) verbatim. □

Chapter 4

Further Applications

In this chapter, we establish additional applications of the locality results shown in Chapter 3 and consider the physical interpretation of these results.

We remark that only the results presented in Sections 4.1 and 4.2 are relevant to the lattice relaxation problem. In particular, we will make use of the estimate Proposition 4.1 shown in Section 4.1 in subsequent chapters.

4.1 Thermodynamic limit estimates

The following result provides an estimate for comparing the infinite ground state with its finite approximation, over compact sets, thus providing explicit rates of convergence for the thermodynamic limit. This is discussed in Remark 8.

Interpreted differently, the result yields estimates on the decay of the perturbation from the bulk electronic structure at a domain boundary, generalising the exponential decay estimate [9, Theorem 4.6] to arbitrary open $\Omega \subset \mathbb{R}^3$ and general $m \in \mathcal{M}_{L^2}(M, \omega)$, in the Coulomb setting.

Proposition 4.1. *Let $m \in \mathcal{M}_{L^2}(M, \omega)$ and (u, ϕ) be the corresponding ground state. Further, let $\Omega \subset \mathbb{R}^3$ be open and suppose there exists $m_\Omega : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$ such that $m_\Omega = m$ on Ω and $\|m_\Omega\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq M$ (e.g., $m_\Omega = m\chi_\Omega$), then there exists (u_Ω, ϕ_Ω) solving (2.2) with $m = m_\Omega$, $u_2 \geq 0$ and $C = C(M, \omega) > 0$,*

$\gamma = \gamma(M, \omega) > 0$, *independent of* Ω, *such that for all* $y \in \Omega$

$$\sum_{|\alpha| \leq 2} |\partial^\alpha (u - u_\Omega)(y)| + |(\phi - \phi_\Omega)(y)| \leq C e^{-\gamma \text{dist}(y, \partial\Omega)}. \tag{4.1}$$

Proposition 4.1 can also be extended to the Yukawa setting.

Proposition 4.2. *Let* $m \in \mathcal{M}_{L^2}(M, \omega)$, $\Omega \subset \mathbb{R}^3$ *be open and suppose there exists* $m_\Omega : \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$ *such that* $m_\Omega = m$ *on* Ω *and* $\|m_\Omega\|_{L^2_{\text{unif}}(\mathbb{R}^3)} \leq M$ *(e.g.,* $m_\Omega = m\chi_\Omega$*). Then there exists* $a_0 = a_0(\omega, m_\Omega) > 0$ *such that for all* $0 < a \leq a_0$ *there exists a ground state* (u_a, ϕ_a) *corresponding to* m *and* $(u_{\Omega,a}, \phi_{\Omega,a})$ *solving* (2.3) *with* $m = m_\Omega$, $u_{\Omega,a} \geq 0$ *and* $C = C(a_0, M, \omega) > 0$, $\gamma = \gamma(a_0, M, \omega) > 0$, *independent of* a *and* Ω, *such that for all* $y \in \Omega$

$$\sum_{|\alpha| \leq 2} |\partial^\alpha (u_a - u_{\Omega,a})(y)| + |(\phi_a - \phi_{\Omega,a})(y)| \leq C e^{-\gamma \text{dist}(y, \partial\Omega)}. \tag{4.2}$$

Remark 8. Let $R > 0$ and $R_n \uparrow \infty$, then applying Proposition 4.1 with $\Omega = B_{R_n}(0)$ and $m_\Omega = m_{R_n}$ gives a rate of convergence for the finite approximation (u_{R_n}, ϕ_{R_n}), solving (2.19), to the ground state (u, ϕ),

$$\|u - u_{R_n}\|_{W^{2,\infty}(B_R(0))} + \|\phi - \phi_{R_n}\|_{L^\infty(B_R(0))} \leq C e^{-\gamma(R_n - R)}.$$

This strengthens the result that (u_{R_n}, ϕ_{R_n}) converges to (u, ϕ) pointwise almost everywhere along a subsequence [16].

Similarly, in the Yukawa case, applying Proposition 4.2, with $\Omega = B_{R_n}(0)$ and $m_\Omega = m_{R_n}$ and $0 < a \leq a_0 = a_0(\omega)$ gives a rate of convergence for the finite approximation $(u_{a,R_n}, \phi_{a,R_n})$, solving (2.3), to the ground state (u_a, ϕ_a)

$$\|u_a - u_{a,R_n}\|_{W^{2,\infty}(B_R(0))} + \|\phi_a - \phi_{a,R_n}\|_{L^\infty(B_R(0))} \leq C e^{-\gamma(R_n - R)}.$$

This strengthens the result that $(u_{a,R_n}, \phi_{a,R_n})$ converges to (u_a, ϕ_a) pointwise almost everywhere along a subsequence [16].

The proof of Proposition 4.1 is an application of Theorem 3.1.

Proof of Proposition 4.1. Observe that $(u_1, \phi_1) = (u, \phi)$ and $(u_2, \phi_2) = (u_\Omega, \phi_\Omega)$ satisfy the conditions of Theorem 3.1, there exist $C, \widetilde{\gamma} > 0$, independent of Ω, such that for all $y \in \mathbb{R}^3$

$$\sum_{|\alpha|\le 2} |\partial^\alpha (u-u_\Omega)(y)|^2 + |(\phi-\phi_\Omega)(y)|^2 \le C \int_{\mathbb{R}^3} |(m-m_\Omega)(x)|^2 e^{-2\gamma|x-y|}\,\mathrm{d}x.$$

Now let $y \in \Omega$, $d = \mathrm{dist}(y, \partial\Omega)$ and observe that $m - m_\Omega \in L^2_{\mathrm{unif}}(\mathbb{R}^3)$. Since $\sup_{x\in A} e^{-2\widetilde{\gamma}|x|} \le C \inf_{x\in A} e^{-2\widetilde{\gamma}|x|}$ for any $A \subset B_1(z), z \in \mathbb{R}^3$, with $C = C(\widetilde{\gamma})$ independent of z, we have the bound

$$\begin{aligned}\int_{B_d(y)^c} &|(m-m_\Omega)(x)|^2 e^{-2\widetilde{\gamma}|x-y|}\,\mathrm{d}x \\ &\le C\left(\|m\|^2_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} + \|m_\Omega\|^2_{L^2_{\mathrm{unif}}(\mathbb{R}^3)}\right)\int_{B_d(y)^c} e^{-2\widetilde{\gamma}|x-y|}\,\mathrm{d}x.\end{aligned}$$

Therefore, we obtain the desired estimate (4.2)

$$\begin{aligned}\int_{\mathbb{R}^3} |(m-m_\Omega)(x)|^2 e^{-2\gamma|x-y|}\,\mathrm{d}x &= \int_{\Omega^c} |(m-m_\Omega)(x)|^2 e^{-2\gamma|x-y|}\,\mathrm{d}x \\ \le \int_{\Omega^c_{\mathrm{buf}}} m(x)^2 e^{-2\widetilde{\gamma}|x-y|}\,\mathrm{d}x &\le CM^2 \int_{\Omega^c_{\mathrm{buf}}} e^{-2\widetilde{\gamma}|x-y|}\,\mathrm{d}x \\ \le CM^2 \int_{B_d(y)^c} e^{-2\widetilde{\gamma}|x-y|}\,\mathrm{d}x &= CM^2(1+d^2)e^{-2\widetilde{\gamma}d} \le CM^2 e^{-2\gamma d},\end{aligned}$$

for any given $0 < \gamma < \widetilde{\gamma}$, where $C = C(\widetilde{\gamma}, \gamma)$. □

Proof of Proposition 4.2. This holds directly from applying Theorem 3.3 and following the proof of Proposition 4.1 verbatim. □

4.2 Neutrality of defects

We use Corollary 3.9 to establish a general result for the neutrality of defects in the TFW model. In models using classical interatomic potentials, it is assumed that the system is composed of atoms, which guarantees the system is charge neutral. In contrast, electronic structure models consider the interaction of charged particles, which in principle allows for non-neutral systems to occur.

Let $m \in \mathcal{M}_{L^2}(M, \omega)$ and $R > 0$, then recall the minimisation problem (2.18) defined in Chapter 2. For finite systems corresponding to

$m_R = m \cdot \chi_{B_R(0)}$, we impose the constraint

$$\int_{\mathbb{R}^3} u_R^2 = \int_{\mathbb{R}^3} m_R, \tag{4.3}$$

which ensures the existence of a minimiser to (2.18). More general charge constraints are treated in [47, Theorems 7.19, 7.23].

When passing to the limit as $R \to \infty$ in (4.3) to the ground state electron density u, as $u \notin L^2(\mathbb{R}^3), m \notin L^1(\mathbb{R}^3)$, it is not possible to claim that $\int_{\mathbb{R}^3} u^2 = \int_{\mathbb{R}^3} m$, i.e. that charge neutrality occurs for general infinite systems. In the specific case of a periodic crystal, charge neutrality is attained as $\int_\Gamma u_{\mathrm{per}}^2 = \int_\Gamma m_{\mathrm{per}}$, where $\Gamma \subset \mathbb{R}^3$ is the unit cell of the crystal.

In [16], the introduction of a local defect $\nu \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ into an otherwise perfect crystal is considered, and it is shown that the residual charge density $\rho_\nu \in L^2(\mathbb{R}^3)$ satisfies a weak form of the neutrality condition $\widehat{\rho}_\nu(0) = 0$, where $\widehat{\rho}_\nu$ denotes the Fourier transform of ρ_ν. This result can be interpreted as stating that it is not possible for a local defect to introduce a charge into a perfect crystal in the TFW model. However, without showing that $\rho_\nu \in L^1(\mathbb{R}^3)$, it does not necessarily follow that $\int_{\mathbb{R}^3} \rho_\nu = 0$.

We now generalise and strengthen the result of [16] by considering the introduction of a defect to a general nuclear configuration $m \in \mathcal{M}_{L^2}(M, \omega)$. Moreover, we also show that if the defect term satisfies certain decay assumptions, we may also estimate the decay of charges away from the defect core.

An immediate consequence of Corollary 3.9 is the neutrality of nuclear perturbations in the TFW equations. This result applies to all nuclear configurations belonging to $\mathcal{M}_{L^2}(M, \omega)$. In particular Theorem 4.3(3) strengthens the result of [14], which requires $m_1 - m_2 \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ and thus excludes typical point defects; see Remark 10 for more details.

In the following result, other than a differing constant, the statement of the result is identical for the Coulomb and Yukawa models.

Let $k > 0$ and $m_1, m_2 \in \mathcal{M}_{L^2}(M, \omega)$.

(C) Let $(u_1, \phi_1), (u_2, \phi_2)$ denote the corresponding Coulomb ground states.

(Y) Let $a_0 > 0$ and for $0 < a \leq a_0$, let $(u_1, \phi_1) = (u_{1,a_1}, \phi_{1,a_1})$ and $(u_2, \phi_2) = (u_{2,a_2}, \phi_{2,a_2})$ denote the corresponding Yukawa ground states.

In addition, for both (C) and (Y), define the residual charge density when comparing the ground states (u_1, ϕ_1) and (u_2, ϕ_2),

$$\rho_{12} = m_1 - u_1^2 - m_2 + u_2^2.$$

If one considers m_2 as a perturbation of the nuclear arrangement m_1, then $\int_{\mathbb{R}^3} \rho_{12}$ represents the charge due to the response of the ground state. The following theorem describes the decay properties of local residual charge integrals. In addition, the result also provides conditions ensuring that $\int_{\mathbb{R}^3} \rho_{12} = 0$, which implies that no charge is introduced by the perturbation.

Theorem 4.3. *Suppose that either* (C) *or* (Y) *holds.*

1. *If there exist* $C, \widetilde{\gamma} > 0$ *such that* $|(m_1 - m_2)(x)| \leq Ce^{-\widetilde{\gamma}|x|}$, *then* $\rho_{12} \in L^1(\mathbb{R}^3)$ *and there exist* $C = C_C(\widetilde{\gamma}, M, \omega), \gamma = \gamma_C(\widetilde{\gamma}, M, \omega) > 0$ *or* $C = C_Y(a_0, \widetilde{\gamma}, M, \omega), \gamma = \gamma_Y(a_0, \widetilde{\gamma}, M, \omega) > 0$, *such that for all* $R > 0$,

$$\left| \int_{B_R(0)} \rho_{12} \right| \leq Ce^{-\gamma R}. \tag{4.4}$$

   Moreover, as $\rho_{12} \in L^1(\mathbb{R}^3)$, *it follows that* $\int_{\mathbb{R}^3} \rho_{12} = 0$.

2. *If there exists* $C, r > 0$ *such that* $|(m_1 - m_2)(x)| \leq C(1 + |x|)^{-r}$ *then there exist* $C = C_C(r, M, \omega)$ *or* $C = C_Y(a_0, r, M, \omega) > 0$, *such that for all* $R > 0$,

$$\left| \int_{B_R(0)} \rho_{12} \right| \leq C(1 + R)^{2-r}. \tag{4.5}$$

   In particular, if $r > 3$ *then* $\rho_{12} \in L^1(\mathbb{R}^3)$, *hence* $\int_{\mathbb{R}^3} \rho_{12} = 0$.

3. *If* $m_1 - m_2 \in L^2(\mathbb{R}^3)$ *(e.g.,* $r > 3/2$ *in* (2)*) then* $\rho_{12} \in L^2(\mathbb{R}^3)$ *and*

$$\lim_{\varepsilon \to 0} \frac{1}{|B_\varepsilon(0)|} \int_{B_\varepsilon(0)} \widehat{\rho}_{12}(k) \, \mathrm{d}k = 0, \tag{4.6}$$

   where $\widehat{\rho}_{12}$ *denotes the Fourier transform of* ρ_{12}.

Remark 9. Consider the case when $m_1 = m_{\text{per}}$ represents the nuclear configuration of a perfect crystal $\mathbb{Z}^3$ with a unit cell $\Gamma \subset \mathbb{R}^3$. By construction, the periodic system satisfies $\int_{\Gamma+k} m_{\mathrm{per}} = \int_{\Gamma+k} u_{\mathrm{per}}^2$, for all $k \in \mathbb{Z}^3$. Further, suppose m_2 satisfies (1) or (2) with $r > 3$, so that $\rho_{12} \in L^1(\mathbb{R}^3)$. It follows that a weak form of the neutrality condition (4.3) holds for the system (m_2, u_2, ϕ_2) as

$$\sum_{k\in\mathbb{Z}^3} \int_{\Gamma+k} (m_2 - u_2^2) = \sum_{k\in\mathbb{Z}^3} \int_{\Gamma+k} \rho_{12} = \int_{\mathbb{R}^3} \rho_{12} = 0.$$

Without showing that $m_2 - u_2^2 \in L^1(\mathbb{R}^3)$, it is not currently possible to conclude that $\int_{\mathbb{R}^3}(m_2 - u_2^2) = 0$.

Remark 10. In Chapter 6, we construct a variational problem to study the response of a crystal due to a local defect, using the TFW energy. Our main result Theorem 6.5 states that any minimising displacement decays away from the defect at the rate $|x|^{-2}$, which corresponds to case (2) with $r = 2$. In this case (4.5) only provides a uniform bound for the charge as opposed to a decay estimate. However, as $r > 3/2$ the global neutrality result (4.6) holds for the relaxed system.

The neutrality estimates of Theorem 4.3 strengthen those of [14] in the following ways. Firstly, our result considers a perturbation of a general nuclear arrangement as opposed to a perfect crystal. This allows us, in [2], to consider the response of extended defects such as dislocations. In addition, we only require that the nuclear perturbation belongs to $L^2(\mathbb{R}^3)$, which we prove rigorously in Chapter 6, whereas in [14] the nuclear defect is assumed to lie in $L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$, which fails for typical point defects. $\square$

Proof of Theorem 4.3. Recall that $\rho_{12} = m_1 - u_1^2 - m_2 + u_2^2$. Let $R > 0$ and choose $\varphi_R \in C_c^\infty(\mathbb{R}^3)$ satisfying $0 \leq \varphi_R \leq 1$, $\varphi_R = 1$ on $B_R(0)$, $\varphi_R = 0$ outside $B_{R+1}(0)$ and $\|\varphi_R\|_{W^{2,\infty}(\mathbb{R}^3)} \leq c_\varphi$. Let $A_R := B_{R+1}(0) \setminus B_R(0)$.

First suppose that (C) holds and recall (3.23b), that the difference $\psi = \phi_1 - \phi_2$ solves

$$-\Delta\psi = 4\pi\rho_{12} \tag{4.7}$$

pointwise. Testing (4.7) with φ_R and using integration by parts yields

$$\int_{B_{R+1}(0)} \rho_{12}\varphi_R = -\frac{1}{4\pi}\int_{A_R} \psi\Delta\varphi_R.$$

Since $\varphi_R = 1$ on $B_R(0)$, we deduce

$$\int_{B_R(0)} \rho_{12} = -\frac{1}{4\pi}\int_{A_R} \psi\Delta\varphi_R - \int_{A_R} \rho_{12}\varphi_R,$$

and as $u_1, u_2 \in L^\infty(\mathbb{R}^3)$ by Proposition 2.1, hence

$$\left|\int_{B_R(0)} \rho_{12}\right| \leq C\int_{A_R} \left(|m_1 - m_2| + |u_1 - u_2| + |\phi_1 - \phi_2|\right), \tag{4.8}$$

where $C = C(c_\varphi, M, \omega) > 0$ is independent of R. Observe that $|A_R| \leq CR^2$.

When (Y) holds, the difference ψ instead solves

$$-\Delta\psi + a^2\psi = 4\pi\rho_{12} \tag{4.9}$$

pointwise. Testing (4.9) with φ_R and rearranging gives

$$\int_{B_R(0)} \rho_{12} = -\frac{1}{4\pi}\int_{A_R} \psi\Delta\varphi_R + \frac{a^2}{4\pi}\int_{A_R} \psi\varphi_R - \int_{A_R} \rho_{12}\varphi_R,$$

so the estimate (4.8) continues to hold, where the constant C now depends on c_φ and a_0. From this point on, the proofs in the cases (C) or (Y) are identical.

(1) By (3.69) of Corollary 3.9 there exists $C, \widetilde{\gamma} > 0$ such that

$$|(\phi_1 - \phi_2)(x)| + |(m_1 - m_2)(x)| + |(u_1 - u_2)(x)| \leq Ce^{-\widetilde{\gamma}|x|}.$$

Then using (4.8) we deduce

$$\begin{aligned}\left|\int_{B_R(0)} \rho_{12}\right| &\leq C\int_{A_R} \left(|m_1 - m_2| + |u_1 - u_2| + |\phi_1 - \phi_2|\right)\\ &\leq C\int_{A_R} e^{-\widetilde{\gamma}|x|}\,\mathrm{d}x \leq C(1 + R^2)e^{-\widetilde{\gamma}R},\end{aligned}$$

which implies (4.4) for any $0 < \gamma < \widetilde{\gamma}$.

(2) Suppose now that $|(m_1 - m_2)(x)| \leq C(1 + |x|)^{-r}$, then using (3.70) and (4.8) we obtain

$$\left|\int_{B_R(0)} \rho_{12}\right| \leq C\int_{A_R} (1 + |x|)^{-r} \leq C(1 + R)^{2-r}.$$

(3) Suppose $m_1 - m_2 \in L^2(\mathbb{R}^3)$, then by Corollary 3.9 we have that $u_1 - u_2, \phi_1 - \phi_2 \in H^2(\mathbb{R}^3)$, hence by Proposition 2.1 $u_1^2 - u_2^2 \in L^2(\mathbb{R}^3)$. Taking the Fourier transform, $\widehat{f}(k) = \int_{\mathbb{R}^3} f(x) e^{-2\pi i k \cdot x}\, \mathrm{d}x$, of (4.7) and rearranging gives

$$\frac{\widehat{\rho}_{12}(k)}{|k|^2} = \pi \widehat{\psi}(k) \in L^2(\mathbb{R}^3).$$

Arguing as in [14] we show that 0 is a Lebesgue point for $\widehat{\rho}_{12}$. For $\varepsilon > 0$,

$$\begin{aligned}\frac{1}{|B_\varepsilon(0)|} \int_{B_\varepsilon(0)} |\widehat{\rho}_{12}(k)|\, \mathrm{d}k &\leq \frac{1}{|B_\varepsilon(0)|} \left(\int_{B_\varepsilon(0)} |k|^4\, \mathrm{d}k \right)^{1/2} \left(\int_{B_\varepsilon(0)} \frac{|\widehat{\rho}_{12}(k)|^2}{|k|^4}\, \mathrm{d}k \right)^{1/2} \\ &\leq C \varepsilon^{1/2} \|\phi_1 - \phi_2\|_{L^2(\mathbb{R}^3)},\end{aligned}$$

which tends to 0 as $\varepsilon \to 0$, as claimed. $\square$

4.3 Impurity screening

The estimate (3.69) from Corollary 3.9 can be used to study the full non-linear response of the ground state to a nuclear impurity, in the Coulomb setting. We compare this to the results from the Thomas–Fermi (TF) [3, 39, 59] and TFW [21, 53, 61, 41] theories of screening with the Coulomb interaction. We remark that similar results also hold in the Yukawa setting.

Consider a nuclear arrangement $m_1 \in \mathcal{M}_{L^2}(M, \omega)$ and model a nuclear impurity at the origin with positive charge Z by $Z\eta(x)$, where $\eta \in C_c^\infty(\mathbb{R}^3)$, $\eta \geq 0$ and $\int \eta = 1$. Then define the perturbed system by $m_2 = m_1 + Z\eta \in \mathcal{M}_{L^2}(M_1, \omega_1)$ and consider the corresponding TFW ground states (u_1, ϕ_1) and (u_2, ϕ_2), respectively. From (3.69) of Corollary 3.9 it follows that

$$\sum_{|\alpha| \leq 2} |\partial^\alpha (u_1 - u_2)(x)| + |(\phi_1 - \phi_2)(x)| \leq C Z e^{-\gamma |x|}, \tag{4.10}$$

We now compare (4.10) with existing results from the TF and TFW theories of screening. These models consider the formal linear response (n, V) of the electron density and potential to a nuclear impurity at the origin, modelled by the Dirac distribution $Z\delta_0$, in a uniform electron gas. In both models, V satisfies the linear equation

$$-\Delta V = 4\pi[n + Z\delta_0],$$

while n solves either the linearised TF or TFW equations. In the TF model, V and n are shown to satisfy [39, Page 112], [3, Page 342]

$$V(x) = Z\frac{e^{-k_s|x|}}{|x|}, \qquad n(x) = -\frac{Zk_s^2}{4\pi}\frac{e^{-k_s|x|}}{|x|}, \tag{4.11}$$

where $k_s > 0$ is a material-dependent constant called the inverse screening length. In the TFW model, V and n satisfy [21, 61, 41, 53]

$$\begin{aligned} V(x) &= \frac{Z}{4\alpha\beta|x|}e^{-\alpha|x|}\left((\alpha+\beta)^2 e^{\beta|x|} - (\alpha-\beta)^2 e^{-\beta|x|}\right), \\ n(x) &= -\frac{(\alpha^2-\beta^2)^2 Z}{\alpha\beta|x|}e^{-\alpha|x|}\left(e^{\beta|x|} - e^{-\beta|x|}\right), \end{aligned} \tag{4.12}$$

where $\alpha \in \mathbb{R}, \beta \in \mathbb{C}$ satisfy $0 < |\beta| < \alpha$. The constants α, β depend on the material and the coefficient C_W, which appears in the definition of the TFW energy (2.1). There is a critical value of C_W below which $\beta > 0$ and above which β is complex, the latter case introduces oscillations in the potential and electron density. In either case, both the TF and TFW models exhibit screening due to the presence of the exponential term appearing in (4.11)–(4.12).

The lack of a factor of the form $\frac{1}{|x|}$ in (4.10) can be attributed to using a smeared nuclear description for the impurity as opposed to a point description in (4.11)–(4.12). Other than this, the similarity of (4.10) to (4.11) suggests that the constant γ in (4.10) may be interpreted as the inverse screening length. In this work we show there exists $\gamma > 0$ satisfying (4.10), however we do not provide any estimates for its value.

The estimate (4.10) shows that screening occurs in the TFW model, without any approximations made to the model and without any restrictions on the nuclear configurations (other than (H1)–(H2)). It should be noted that although (4.10) agrees with existing results from the TF theory of screening, in metals often the effects of screening are weaker. For metals, instead of an exponentially decaying screening factor, Friedel oscillations are observed [27, 52, 36]. In this case, the screening factor behaves as $|x|^{-r} f(|x|)$, where $f : \mathbb{R}_{\geq 0} \to [-1, 1]$ is an oscillating function and the decay rate $r > 0$ depends on the Fermi surface of the metal. The *generic* exponential screening factor in (4.10) demonstrates that the TFW model significantly overscreens charges.

4.4 Convergence from Yukawa to Coulomb

The main result of this section is a uniform estimate comparing the Yukawa and Coulomb ground states corresponding to the same nuclear configuration. This result is essentially a consequence of Theorems 3.1 and 3.2.

In the following, $(u, \phi) = (u_0, \phi_0)$ denotes the corresponding Coulomb ground state solving (2.2), i.e the ground state with Yukawa parameter $a = 0$.

Theorem 4.4. *Suppose $a_0 > 0$, $k \in \mathbb{N}_0$, $m \in \mathcal{M}_{H^k}(M, \omega)$ and let (u, ϕ) denote the corresponding Coulomb ground state. For $0 < a \leq a_0$, let (u_a, ϕ_a) denote the corresponding Yukawa ground state, then there exists a constant $C = C(a_0, k, M, \omega) > 0$ such that*

$$\|u_a - u\|_{W^{k+2,\infty}(\mathbb{R}^3)} + \|\phi_a - \phi\|_{W^{k+2,\infty}(\mathbb{R}^3)} \leq Ca^2. \tag{4.13}$$

Remark 11. The error term in (4.13) arises from the additional term in the Yukawa equation (2.3b), as opposed to due to a difference in nuclear distributions in Theorems 3.1 and 3.2. For this reason, we believe an analogous result to Theorem 4.4 also holds for point charge nuclei. □

Proof of Theorem 4.4. As $m \in \mathcal{M}_{H^k}(M, \omega)$, applying Lemma 3.8(B) with $a_1 = 0$ and $0 < a_2 = a \leq a_0$ and $R = a^2 \phi_2 \in H^{k+2}_{\text{unif}}(\mathbb{R}^3)$. Then applying the estimate (3.58) of Lemma 3.8(B) with $\xi(x) = e^{-\gamma|x-y|} \in H_\gamma$ yields

$$\sum_{|\alpha| \leq k+2} \left(|\partial^\alpha w(y)|^2 + |\partial^\alpha \psi(y)|^2\right) \leq Ca^2 \int_{\mathbb{R}^3} \sum_{|\beta| \leq k+2} |\partial^\beta \phi_2(x)|^2 e^{-2\gamma|x-y|} \, \mathrm{d}x.$$

As $\phi_2 \in H^{k+2}_{\text{unif}}(\mathbb{R}^3)$, and for all $z \in \mathbb{R}^3$ and $A \subset B_1(z)$,

$\sup_{x\in A} e^{-2\gamma|x|} \le C \inf_{x\in A} e^{-2\gamma|x|}$, it follows that

$$\begin{aligned}\sum_{|\alpha|\le k+2} \left(|\partial^\alpha w(y)|^2 + |\partial^\alpha \psi(y)|^2\right) &\le Ca^2 \int_{\mathbb{R}^3} \sum_{|\beta|\le k+2} |\partial^\beta \phi_2(x)|^2 e^{-2\gamma|x-y|} \, \mathrm{d}x \\ &\le Ca^2 \|\phi_2\|^2_{H^{k+2}_{\mathrm{unif}}(\mathbb{R}^3)} \int_{\mathbb{R}^3} e^{-2\gamma|x-y|} \, \mathrm{d}x \\ &\le Ca^2,\end{aligned}$$

where C is independent of $y \in \mathbb{R}^3$, hence the desired estimate (4.13) holds. $\square$

Chapter 5

Energy and Force Locality

In this chapter, we show that the locality result, Theorem 3.2, can be used to describe the energy contribution of each individual nucleus. In effect, we will derive a *site energy potential* for the TFW model, which has the surprising consequence that, for the study of mechanical response, TFW can be treated as a classical short-ranged interatomic potential. Our result gives credence to the construction of interatomic potentials and the assumption of *strong locality* used in hybrid quantum mechanics/molecular mechanics (QM/MM) simulations [19].

The main idea of QM/MM simulations of a quantum system is to separate the system into small regions where a highly accurate quantum description is required, hence more expensive methods such as Kohn Sham or DFT are used, and the remainder of the system where cheaper and faster methods are more efficient, such as empirical atomistic potentials. To successfully apply these methods, it is important that the interaction of particles in the quantum regions is short-ranged, that is, rapidly decreasing as the distance between the particles tends to infinity. The idea of strong locality is used to describe this condition [19]: if E describes the total energy of a quantum system depending on atoms positioned at $Y_i \in \mathbb{R}^3$, indexed by $i \in \mathbb{N}$, then strong locality holds if

$$\frac{\partial^2 E(Y)}{\partial Y_i \partial Y_j} \to 0 \text{ sufficiently rapidly as } |Y_i - Y_j| \to \infty, \ \forall i, j \in \mathbb{N} \text{ such that } i \neq j.$$

Our notion of force locality matches the definition of strong locality given above, and we will in fact show that the forces decay exponentially with distance in the TFW model. Using this, we also decompose the total TFW energy into local contributions that can each be associated to an individual nucleus in the arrangement. This decomposition of the energy will be essential in our analysis of the lattice relaxation problem presented in Chapter 6.

5.1 Construction of site energies

Let $\eta \in C_c^\infty(B_{R_0}(0))$ be a radially symmetric function satisfying $\eta \geq 0$ and $\int_{\mathbb{R}^3} \eta = 1$ describes the charge density of a single (smeared) nucleus, for some fixed $R_0 > 0$. For any countable collection of nuclear coordinates
$Y = (Y_j)_{j\in\mathbb{N}} \in (\mathbb{R}^3)^{\mathbb{N}}$, let the corresponding nuclear configuration be defined by

$$m_Y(x) = \sum_{j\in\mathbb{N}} \eta(x - Y_j). \tag{5.1}$$

A natural space of nuclear coordinates, related to the $\mathcal{M}_{L^2}$ space is

$$\mathcal{Y}_{L^2}(M,\omega) := \{\, Y \in (\mathbb{R}^3)^{\mathbb{N}} \,|\, m_Y \in \mathcal{M}_{L^2}(M,\omega) \,\}.$$

One could similarly define $\mathcal{Y}_{H^k}(M,\omega)$ related to the space $\mathcal{Y}_{H^k}(M,\omega)$, however using these spaces would not yield any significant results.

We now show that there exists $R' = R'(R_0,\omega) > 0$ such that for any $Y \subset \mathcal{Y}_{L^2}(M,\omega)$

$$\bigcup_{j\in\mathbb{N}} B_{R'}(Y_j) = \mathbb{R}^3. \tag{5.2}$$

As $m_Y \in \mathcal{M}_{L^2}(M,\omega)$, there exists $R_1 = R_1(\omega) > 0$ such that

$$\inf_{x\in\mathbb{R}^3} \int_{B_{R_1}(x)} m_Y(z)\,\mathrm{d}z \geq 1 > 0,$$

hence by the definition (5.1), we deduce that for every $x \in \mathbb{R}^3$, there exists $j \in \mathbb{N}$ such that $B_{R_1}(x) \cap B_{R_0}(Y_j) \neq \emptyset$, in particular $|x - Y_j| \leq R_1 + R_0 =: R'$ and hence (5.2) holds.

For any $Y \in \mathcal{Y}_{L^2}(M, \omega)$ there exists a unique ground state (u, ϕ) corresponding to $m = m_Y$. Naively, we might define a corresponding energy density by

$$\mathcal{E}(Y; x) := |\nabla u(x)|^2 + u(x)^{10/3} + \frac{1}{2}\left((m - u^2) * \tfrac{1}{|\cdot|}\right)(x)(m - u^2)(x), \quad (5.3)$$

however, difficulties arise due to the fact that $(m - u^2) * \frac{1}{|\cdot|}$ is not well defined. Instead, we give two alternative definitions for the energy density for an infinite system:

$$\mathcal{E}_1(Y; x) := |\nabla u(x)|^2 + u(x)^{10/3} + \frac{1}{2}\phi(x)(m - u^2)(x), \quad (5.4)$$

$$\mathcal{E}_2(Y; x) := |\nabla u(x)|^2 + u(x)^{10/3} + \frac{1}{8\pi}|\nabla \phi(x)|^2, \quad (5.5)$$

which both satisfy $\mathcal{E}_1(Y; \cdot), \mathcal{E}_2(Y; \cdot) \in L^1_{\mathrm{unif}}(\mathbb{R}^3)$.

Suppose now that $\Omega \subset \mathbb{R}^3$ is a charge-neutral volume [66], that is, if n is the unit normal to $\partial\Omega$, then $\nabla\phi \cdot n = 0$ on $\partial\Omega$. Recalling from (2.2b) that

$$-\Delta\phi = 4\pi(m - u^2)$$

we deduce that

$$\frac{1}{8\pi}\int_\Omega |\nabla\phi|^2 = \frac{1}{8\pi}\int_\Omega (-\Delta\phi)\phi + \int_{\partial\Omega} \phi\nabla\phi \cdot n = \frac{1}{2}\int_\Omega \phi(m - u^2),$$

and hence

$$\int_\Omega \mathcal{E}_1(Y; x)\, \mathrm{d}x = \int_\Omega \mathcal{E}_2(Y; x)\, \mathrm{d}x.$$

In particular, for finite neutral systems and $\Omega = \mathbb{R}^3$, we obtain that the three energies (5.3), (5.4) and (5.5) agree. This claim is made precise in Lemma 5.4. Thus, we have derived two energy densities, $\mathcal{E}_1, \mathcal{E}_2$, which are meaningful and well-defined also for infinite configurations.

In order to define site energies, we require a partition of $\mathbb{R}^3$. For each $j \in \mathbb{N}$ let $\varphi_j(Y; \cdot) \in C^1(\mathbb{R}^3), \varphi_j(Y; \cdot) \geq 0$ satisfying the following conditions:

there exist $C, \widetilde{\gamma} > 0$ such that for all $Y \in \mathcal{Y}_{L^2}(M,\omega)$ and $n \in \mathbb{N}$

$$\sum_{j\in\mathbb{N}} \varphi_j(Y;x) = 1, \tag{5.6a}$$

$$|\varphi_j(Y;x)| \leq Ce^{-\widetilde{\gamma}|x-Y_j|}, \quad \text{and} \tag{5.6b}$$

$$\left|\frac{\partial \varphi_j}{\partial Y_n}(Y;x)\right| \leq Ce^{-\widetilde{\gamma}|x-Y_j|}e^{-\widetilde{\gamma}|x-Y_n|}. \tag{5.6c}$$

We propose a canonical construction of such a partition in Remark 12 below.

Given a family of partition functions satisfying (5.6), we can define site energies

$$E_j^{(i)}(Y) = \int_{\mathbb{R}^3} \mathcal{E}_i(Y;x)\varphi_j(Y;x)\,\mathrm{d}x, \tag{5.7}$$

for $i = 1,2$. A consequence of Theorems 3.1 and 3.2 is that $E_j^{(i)}(Y)$ are *local*: their dependence on the environment of nuclei decays exponentially fast. This is made precise in the following theorem, which is the main result of this chapter.

Theorem 5.1. *Let $i \in \{1,2\}$, $Y \in \mathcal{Y}_{L^2}(M,\omega)$ and $\{\varphi_j | j \in \mathbb{N}\}$ satisfy (5.6). Then for every $n \in \mathbb{N}$, $\partial_{Y_n} E_j^{(i)}$ exists and satisfies*

$$\left|\frac{\partial E_j^{(i)}(Y)}{\partial Y_n}\right| \leq Ce^{-\gamma|Y_j-Y_n|}, \tag{5.8}$$

where $C = C(M,\omega)$, $\gamma = \gamma(M,\omega) > 0$.

The derivative $\partial_{Y_n} E_j^{(i)}$ can be interpreted as the contribution of the atom at Y_n to the force on the nucleus at Y_j. In addition, we show on Page 148 in Section 5.6 that these site energies generate the correct total force

$$\sum_{j\in\mathbb{N}} \frac{\partial E_j^{(1)}(Y)}{\partial Y_n} = \sum_{j\in\mathbb{N}} \frac{\partial E_j^{(2)}(Y)}{\partial Y_n} = \int_{\mathbb{R}^3} \phi(x)\,\frac{\partial m_Y(x)}{\partial Y_n}\,\mathrm{d}x. \tag{5.9}$$

After introducing the idea of taking derivatives of a function with respect to the nuclear coordinates, we prove and generalise Theorem 5.1 to higher derivatives for site energies in Section 5.6.

Remark 12. Two further canonical requirements on a site energy potential are permutation and isometry (rotation and translation) invariance. This can be obtained as follows:

If the partition $(\varphi_j)_{j\in\mathbb{N}}$ is *permutation invariant*, that is, for any bijection $P : \mathbb{N} \to \mathbb{N}$, $Y \circ P = (Y_{P(j)})_{j\in\mathbb{N}}$, we have

$$\varphi_j(Y \circ P; x) = \varphi_{P(j)}(Y; x) \qquad \forall\, j \in \mathbb{N} \quad x \in \mathbb{R}^3, \tag{5.10}$$

then so are the site energies,

$$E_j^{(i)}(Y \circ P) = E_{P(j)}^{(i)}(Y).$$

If the partition is *isometry invariant*, that is, for any isometry $A : \mathbb{R}^3 \to \mathbb{R}^3$, $AY = (AY_j)_{j\in\mathbb{N}}$, we have

$$\varphi_j(AY; x) = \varphi_j(Y; A^{-1}x) \qquad \forall\, j \in \mathbb{N}, \quad x \in \mathbb{R}^3, \tag{5.11}$$

then the site energies are also isometry invariant,

$$E_j^{(i)}(AY) = E_j^{(i)}(Y).$$

Both statements are proved in Lemma 5.5 in Section 5.3. A canonical class of partitions satisfying (5.6) as well as (5.10), (5.11) can be constructed as follows: let $\widetilde{\varphi} \in C^1(\mathbb{R}^3)$, $\widetilde{\varphi} \geq 0$, be radially symmetric and satisfy

$$\begin{aligned} &|\widetilde{\varphi}(x)| + |\nabla\widetilde{\varphi}(x)| \leq Ce^{-\widetilde{\gamma}|x|}, \\ &\widetilde{\varphi}(x) \geq c > 0 \qquad \text{on } B_{R'+1}(0). \end{aligned}$$

For example, this holds for $\widetilde{\varphi}(x) = e^{-\gamma|x|^2}$ for $0 < \widetilde{\gamma} < \gamma$ and for standard mollifiers with sufficiently wide support.

Then, for $j \in \mathbb{N}$, we can define

$$\varphi_j(Y; x) = \frac{\widetilde{\varphi}(x - Y_j)}{\sum_{j'\in\mathbb{N}} \widetilde{\varphi}(x - Y_{j'})}.$$

It is easy to see that this class of functions are well-defined and satisfies all requirements, including (5.84) for all $k \in \mathbb{N}$. $\square$

Remark 13. Alternative constructions of energy partitions include Bader volumes and charge-neutral volumes [5, 66, 51]. Bader volumes partition space into regions such that the flux of the electron density on the boundary is zero, while charge-neutral volumes are defined so that each region has zero charge. The construction of these volumes is not unique, like our definition of a partition. Bader volumes were developed as a means to define atoms within molecules [5].

With this in mind, using a partition we may assign a portion of the electron density to each nucleus in the system. We refer to a nucleus paired with its associated partition of the electron density as an effective atom. Due to the screening that occurs in the TFW model, the interaction of two effective atoms decays exponentially as the distance between the nuclei grows. In comparison, the interaction of two neutral atoms separated by a sufficiently large distance r in the TF model has been shown to decay at the rate r^{-7} [12]. This suggests that due to the overscreening of the TFW model, the interaction of the effective atoms is considerably weaker than is realistic. However, for the purpose of simulating quantum systems, in particular applying the strong locality principle [19], the weak long-range interaction of the TFW model is a desirable property. $\square$

5.2 Convergence of Yukawa forces

We now consider using the TFW Yukawa model to define energy densities corresponding to infinite systems.

For $Y \in \mathcal{Y}_{L^2}(M,\omega)$ and $a > 0$ there exists a unique Yukawa ground state (u_a, ϕ_a) corresponding to $m = m_Y$. We give two definitions for the Yukawa energy density for an infinite system:

$$\mathcal{E}_{1,a}(Y;x) := |\nabla u_a(x)|^2 + u_a(x)^{10/3} + \frac{1}{2}\phi_a(x)(m - u_a^2)(x), \tag{5.12}$$

$$\mathcal{E}_{2,a}(Y;x) := |\nabla u_a(x)|^2 + u_a(x)^{10/3} + \frac{1}{8\pi}\left(|\nabla \phi_a(x)|^2 + a^2\phi_a(x)^2\right). \tag{5.13}$$

These satisfy $\mathcal{E}_{1,a}(Y;\cdot), \mathcal{E}_{2,a}(Y;\cdot) \in L^1_{\mathrm{unif}}(\mathbb{R}^3)$. As the definitions of (5.12)–

(5.13) are analogous those of the Coulomb energy densities (5.4)–(5.5), the argument presented in the Coulomb setting can be applied verbatim to show that the two energies agree when Ω is a charge-neutral volume and also for finite systems when $\Omega = \mathbb{R}^3$.

The following result shows that the force generated by a nucleus in the Yukawa setting is well defined and converges when passing from the Yukawa to the Coulomb setting by sending $a \to 0$. This is an application of Theorem 4.4, which shows the uniform convergence of ground states from the Yukawa to the Coulomb model.

Theorem 5.2. *Let $a_0 > 0$, $Y \in \mathcal{Y}_{L^2}(M, \omega)$ and $i \in \{1, 2\}$, then for all $0 < a \leq a_0$ and $k \in \mathbb{N}$, the Yukawa force density $\partial_{Y_k} \mathcal{E}_{i,a}(Y, \cdot) \in L^1(\mathbb{R}^3)$ exists and satisfies*

$$\int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_{1,a}}{\partial Y_k}(Y; x)\, \mathrm{d}x = \int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_{2,a}}{\partial Y_k}(Y; x)\, \mathrm{d}x = \int_{\mathbb{R}^3} \phi_a(x) \frac{\partial m_Y(x)}{\partial Y_k}\, \mathrm{d}x. \tag{5.14}$$

In addition, the Coulomb force density $\partial_{Y_k} \mathcal{E}_i(Y, \cdot) \in L^1(\mathbb{R}^3)$ also exists and there exists $C = C(a_0, M, \omega) > 0$ such that for all $0 < a \leq a_0$

$$\left| \int_{\mathbb{R}^3} \left(\frac{\partial \mathcal{E}_{i,a}}{\partial Y_k} - \frac{\partial \mathcal{E}_i}{\partial Y_k} \right) (Y; x)\, \mathrm{d}x \right| \leq C a^2. \tag{5.15}$$

The expression (5.14) shows that the forces generated by the energy densities $\mathcal{E}_{1,a}$ and $\mathcal{E}_{2,a}$ are identical. Also, (5.15) establishes an $O(a^2)$ convergence of forces when passing from the Yukawa to the Coulomb model. The proof of Theorem 5.2 can be found on Page 151 in Section 5.6.

5.3 Preliminary results

In the following, let $\mathbb{R}^3_* = \mathbb{R}^3 \setminus \{0\}$. Now fix $Y = (Y_j)_{j \in \mathbb{N}} \in \mathcal{Y}_{L^2}(M, \omega)$ and let $m = m_Y \in \mathcal{M}_{L^2}(M, \omega)$. Let $V \in \mathbb{R}^3_*$, $k \in \mathbb{N}$ and for $h \in [0, 1]$ define

$$Y^h = \{\, Y_j + \delta_{jk} h V \mid j \in \mathbb{N} \,\}, \tag{5.16}$$

and the associated nuclear configuration

$$m_h(x) = m(x) + \eta(x - Y_k - hV) - \eta(x - Y_k). \tag{5.17}$$

Lemma 5.3. *There exist $M', \omega_0', \omega_1' > 0$, such that for $\omega' = (\omega_0', \omega_1')$ and $m_h \in \mathcal{M}_{L^2}(M', \omega')$ for all $h \in [0, 1]$. In particular, $Y^h \in \mathcal{Y}_{L^2}(M', \omega')$ for all $h \in [0, 1]$.*

Proof of Lemma 5.3. Recall that $m_h, \eta \geq 0$, $\eta \in C^\infty(\mathbb{R}^3)$ and $\int_{\mathbb{R}^3} \eta = 1$, then

$$\begin{aligned}
\sup_{x \in \mathbb{R}^3} \|m_h\|_{L^2(B_1(x))} &\leq \sup_{x \in \mathbb{R}^3} \left(\|m\|_{L^2(B_1(x))} + \left(\int_{B_1(x)} \eta(z - Y_k - hV)^2 \, \mathrm{d}z \right)^{1/2} \right) \\
&\leq M + \|\eta\|_{L^2(\mathbb{R}^3)} =: M'.
\end{aligned}$$

Since $m \in \mathcal{M}_{L^2}(M, \omega)$, with $\omega = (\omega_0, \omega_1)$, for all $R > 0$,

$$\begin{aligned}
\inf_{x \in \mathbb{R}^3} \int_{B_R(x)} m_h(z) \, \mathrm{d}z &\geq \inf_{x \in \mathbb{R}^3} \int_{B_R(x)} m(z) \, \mathrm{d}z - \int_{B_R(x)} \eta(z - Y_k) \, \mathrm{d}z \\
&\geq \omega_0 R^3 - \omega_1 - 1,
\end{aligned}$$

hence for $\omega' = (\omega_0, \omega_1 + 1)$, $m_h \in \mathcal{M}_{L^2}(M', \omega')$ for all $h \in [0, 1]$, as claimed. $\square$

Lemma 5.4. *For $m \in L^2_{\mathrm{unif}}(\mathbb{R}^3)$ with compact support, let (u, ϕ) denote the corresponding ground state. Then, one may define the following energy densities, analogously to (5.3)–(5.5)*

$$\begin{aligned}
\mathcal{E}(x) &:= |\nabla u(x)|^2 + u(x)^{10/3} + \frac{1}{2} \left((m - u^2) * \tfrac{1}{|\cdot|} \right)(x)(m - u^2)(x), \\
\mathcal{E}_1(x) &:= |\nabla u(x)|^2 + u(x)^{10/3} + \frac{1}{2} \phi(x)(m - u^2)(x), \\
\mathcal{E}_2(x) &:= |\nabla u(x)|^2 + u(x)^{10/3} + \frac{1}{8\pi} |\nabla \phi(x)|^2,
\end{aligned}$$

which satisfy $\mathcal{E}, \mathcal{E}_1, \mathcal{E}_2 \in L^1(\mathbb{R}^3)$ and

$$\int_{\mathbb{R}^3} \mathcal{E}(x) \, \mathrm{d}x = \int_{\mathbb{R}^3} \mathcal{E}_1(x) \, \mathrm{d}x = \int_{\mathbb{R}^3} \mathcal{E}_2(x) \, \mathrm{d}x.$$

Proof of Lemma 5.4. This proof follows the argument used in Proposition 2.11 to show (2.27). As $m \in L^2_{\mathrm{unif}}(\mathbb{R}^3)$ has compact support, it follows that

$m \in L^1(\mathbb{R}^3)$. Consider the variational problem (2.18)

$$I^{\mathrm{TFW}}(m) = \inf\left\{ E^{\mathrm{TFW}}(v, m) \,\middle|\, v \in H^1(\mathbb{R}^3), v \geq 0, \int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m \right\},$$

which has the unique minimiser $u \in H^1(\mathbb{R}^3)$ solving

$$-\Delta u + \frac{5}{3}u^{7/3} - \left((m - u^2) * \tfrac{1}{|\cdot|}\right) u = -\theta u.$$

Here $\theta \in \mathbb{R}$ is the Lagrange multiplier associated with the charge constraint. Subsequently, one can define $\phi = (m - u^2) * \frac{1}{|\cdot|} - \theta$. Following the arguments presented on Page 25 verbatim, we obtain the expression (2.27)

$$\frac{1}{2}\int_{\mathbb{R}^3} \left((m - u^2) * \tfrac{1}{|\cdot|}\right)(m - u^2) = \frac{1}{2}\int_{\mathbb{R}^3} \phi(m - u^2) = \frac{1}{8\pi}\int_{\mathbb{R}^3} |\nabla\phi|^2. \quad (5.18)$$

Further, as $u \in H^1(\mathbb{R}^3) \hookrightarrow L^6(\mathbb{R}^3)$, it follows that as $u \in L^2(\mathbb{R}^3) \cap L^6(\mathbb{R}^3)$, by Hölder's inequality, $u \in L^p(\mathbb{R}^3)$ for all $p \in [2, 6]$. It follows that $u \in L^{10/3}(\mathbb{R}^3)$ hence $\mathcal{E}, \mathcal{E}_1, \mathcal{E}_2 \in L^1(\mathbb{R}^3)$, which together with (5.18) implies that

$$\int_{\mathbb{R}^3} \mathcal{E}(x)\, \mathrm{d}x = \int_{\mathbb{R}^3} \mathcal{E}_1(x)\, \mathrm{d}x = \int_{\mathbb{R}^3} \mathcal{E}_2(x)\, \mathrm{d}x.$$

$\square$

Finally, we establish (5.4)–(5.5): if the partition functions φ_j are invariant under permutations and isometries, then so are the site energies.

Lemma 5.5. *If the partition $(\varphi_j)_{j\in\mathbb{N}}$ is permutation and isometry invariant (5.10)–(5.11), then for $i = 1, 2$, for any bijection $P : \mathbb{N} \to \mathbb{N}$, isometry $A : \mathbb{R}^3 \to \mathbb{R}^3$, $j \in \mathbb{N}$ and $Y \in \mathcal{Y}_{L^2}(M, \omega)$*

$$E_j^{(i)}(Y \circ P) = E_{P(j)}^{(i)}(Y), \quad (5.19)$$

$$E_j^{(i)}(AY) = E_j^{(i)}(Y). \quad (5.20)$$

Proof of Lemma 5.5. Let $Y \in \mathcal{Y}_{L^2}(M, \omega)$ and $m = m_Y$, then as $P : \mathbb{N} \to \mathbb{N}$ is a bijection,

$$m_{Y\circ P}(x) = \sum_{j\in\mathbb{N}} \eta(x - Y_{P(j)}) = \sum_{j\in\mathbb{N}} \eta(x - Y_j) = m_Y(x).$$

Since (2.2) has a unique solution, $(u_Y, \phi_Y) = (u_{Y\circ P}, \phi_{Y\circ P})$. Consequently, for $i = 1, 2$, the energy densities satisfy $\mathcal{E}_i(Y \circ P; \cdot) = \mathcal{E}_i(Y; \cdot)$. Together with (5.11) this implies (5.19).

We now show isometry invariance (5.20). First consider a translation $A_1(x) = x + c$, for $c \in \mathbb{R}^3$, then

$$m_{A_1Y}(x) = \sum_{j\in\mathbb{N}} \eta(x - Y_j - c) = m_Y(x - c) = m_Y(A_1^{-1}(x)).$$

Then, by the uniqueness of the TFW equations, it follows that $(u_{A_1Y}, \phi_{A_1Y})(\cdot) = (u_Y, \phi_Y)(\cdot - c)$, so $\mathcal{E}_i(A_1Y; \cdot) = \mathcal{E}_i(Y; \cdot - c)$ and thus

$$\begin{aligned} E_j^{(i)}(A_1Y) &= \int_{\mathbb{R}^3} \mathcal{E}_i(A_1Y; x)\varphi_j(A_1Y; x)\,\mathrm{d}x = \int_{\mathbb{R}^3} \mathcal{E}_i(Y; x - c)\varphi_j(Y; x - c)\,\mathrm{d}x \\ &= \int_{\mathbb{R}^3} \mathcal{E}_i(Y; z)\varphi_j(Y; z)\,\mathrm{d}z = E_j^{(i)}(Y). \end{aligned}$$

Similarly, for a rotation $A_2(x) = Rx$, $R \in \mathrm{O}(3)$, since we assumed that η is radially symmetric,

$$\begin{aligned} m_{A_2Y}(x) &= \sum_{j\in\mathbb{N}} \eta(x - RY_j) = \sum_{j\in\mathbb{N}} \eta(R(R^Tx - Y_j)) = \sum_{j\in\mathbb{N}} \eta(R^Tx - Y_j) \\ &= m_Y(R^Tx). \end{aligned} \tag{5.21}$$

As (u_Y, ϕ_Y) solve (2.2)

$$\begin{aligned} -\Delta u_Y + \frac{5}{3}u_Y^{7/3} - \phi_Y u_Y &= 0, \\ -\Delta \phi_Y &= 4\pi(m_Y - u_Y^2), \end{aligned}$$

then by (5.21) and as the Laplacian is invariant under rotations, it follows that

$(u, \phi) = (u_Y, \phi_Y) \circ A_2^{-2}$ solves

$$-\Delta u + \frac{5}{3} u^{7/3} - \phi u = 0,$$
$$-\Delta \phi = 4\pi(m_Y \circ R^T - u^2) = 4\pi(m_{A_2 Y} - u^2),$$

hence the uniqueness of (2.2) implies $(u_{A_2Y}, \phi_{A_2Y}) = (u_Y, \phi_Y) \circ A_2^{-1}$. It follows that $E_i(A_2Y; \cdot) = E_i(Y; R^T \cdot)$, hence as $\det(R) = \pm 1$, a change of variables shows

$$\begin{aligned} E_j^{(i)}(A_2Y) &= \int_{\mathbb{R}^3} \mathcal{E}_i(A_2Y; x)\varphi_j(A_2Y; x) \, \mathrm{d}x = \int_{\mathbb{R}^3} \mathcal{E}_i(Y; R^T x)\varphi_j(Y; R^T x) \, \mathrm{d}x \\ &= \int_{\mathbb{R}^3} \mathcal{E}_i(Y; z)\varphi_j(Y; z) |\det(R)| \, \mathrm{d}z = \int_{\mathbb{R}^3} \mathcal{E}_i(Y; z)\varphi_j(Y; z) \, \mathrm{d}z \\ &= E_j^{(i)}(Y). \end{aligned}$$

As the site energies are invariant under both translations and rotations, they are invariant under all isometries of $\mathbb{R}^3$. □

5.4 Linear response of the TFW equations

In order to prove Theorem 5.1, we first establish the existence, uniqueness and regularity of the solutions to the linearised TFW equations. We now use Corollary 3.9 to rigorously linearise the TFW Coulomb equations.

Similarly, in Section 5.5 we also generalise these results to higher variations of the TFW equations. Terms from higher variations of the TFW equations appear when generalising Theorem 5.1 to higher derivatives of the site energies, which are required to show that the Coulomb lattice problem is well-defined in Chapter 6.

As $m_h \in \mathcal{Y}_{L^2}(M', \omega')$ for all $h \in [0, 1]$, by [16, Theorem 6.10] and Propositions 2.1 and 2.2, there exists a corresponding Coulomb ground state (u_h, ϕ_h). Also, let $(u, \phi) = (u_0, \phi_0)$.

Lemma 5.6. *Let $Y \in \mathcal{Y}_{L^2}(M, \omega)$ and let $m = m_Y \in \mathcal{M}_{L^2}(M, \omega)$. Also, let*

$k \in \mathbb{N}$, $V \in \mathbb{R}^3$ and $h_0 = (1+|V|)^{-1}$. For $h \in [0, h_0]$ define

$$m_h(x) = m(x) + \eta(x - Y_k - hV) - \eta(x - Y_k).$$

1. *There exist $C = C_C(M', \omega')$, $\gamma_0 = \gamma_0(M', \omega') > 0$, independent of h and $|V|$, such that*

$$\sum_{|\alpha| \le 2} \left(|\partial^\alpha (u_h - u)(x)| + |\partial^\alpha (\phi_h - \phi)(x)|\right) + |(m_h - m)(x)| \le Ch|V|e^{-\gamma_0 |x - Y_k|}, \quad (5.22)$$

$$\|u_h - u\|_{H^4(\mathbb{R}^3)} + \|\phi_h - \phi\|_{H^2(\mathbb{R}^3)} \le C\|m_h - m\|_{L^2(\mathbb{R}^3)} \le Ch|V|. \quad (5.23)$$

2. *There exist $\overline{u} \in H^4(\mathbb{R}^3), \overline{\phi} \in H^2(\mathbb{R}^3), \overline{m} \in C_c^\infty(\mathbb{R}^3)$ such that $\frac{u_h - u}{h}, \frac{\phi_h - \phi}{h}$ converge to $\overline{u}, \overline{\phi}$ respectively, weakly in $H^4(\mathbb{R}^3)$ and $H^2(\mathbb{R}^3)$, strongly in $H^3(B_R(0))$ and $H^1(B_R(0))$ for all $R > 0$ and pointwise almost everywhere, along with their derivatives as $h \to 0$. In addition, $\frac{m_h - m}{h}$ converges pointwise to $\overline{m}$.*

   The pair $(\overline{u}, \overline{\phi})$ is the unique solution to the linearised TFW Coulomb equations

$$\begin{aligned} -\Delta \overline{u} + \left(\frac{35}{9} u^{4/3} - \phi\right) \overline{u} - u\overline{\phi} &= 0, \\ -\Delta \overline{\phi} &= 4\pi \left(\overline{m} - 2u\overline{u}\right). \end{aligned}$$

3. *Moreover, $\overline{u}, \overline{\phi}$ and $\overline{m}$ satisfy*

$$\sum_{|\alpha| \le 2} \left(|\partial^\alpha \overline{u}(x)| + |\partial^\alpha \overline{\phi}(x)|\right) + |\overline{m}(x)| \le C|V|e^{-\gamma_0 |x - Y_k|}, \quad (5.25)$$

$$\|\overline{u}\|_{H^4(\mathbb{R}^3)} + \|\overline{\phi}\|_{H^2(\mathbb{R}^3)} \le C\|\overline{m}\|_{L^2(\mathbb{R}^3)}. \quad (5.26)$$

Remark 14. Observe that the pointwise estimate (5.22) is stronger than the estimate (3.8) shown in Theorem 3.1. This additional regularity is necessary in order to prove Theorem 5.1 for the energy density $\mathcal{E}_2$ (5.5), which is defined using $\nabla\phi$. $\square$

Using Lemma 5.6, we can extend Proposition 4.1 to the linearised TFW equations. The following estimate will be useful to establish homogeneity estimates for site energies and will be useful for formulating the lattice relaxation problem in Chapter 6.

In the following, recall that $R_0 > 0$ is a fixed constant satisfying $\mathrm{spt}(\eta) \subset B_{R_0}(0)$.

Lemma 5.7. *Let $Y_1, Y_2 \in \mathcal{Y}_{L^2}(M, \omega)$ and suppose there exists $R > 0$, such that*

$$\{Y_{1,j} \mid |Y_{1,j}| \leq R + R_0\} = \{Y_{2,j} \mid |Y_{2,j}| \leq R + R_0\}. \tag{5.27}$$

For $i = 1, 2$, define $m_i = m_{Y_i}$, and let (u_i, ϕ_i) denote the corresponding ground state. Then let $V \in \mathbb{R}^3_*$ and $j_1 \in \mathbb{N}$ such that $|Y_{1j_1}| \leq R + R_0$, then there exists unique $j_2 \in \mathbb{N}$ such that $Y_{1j_1} = Y_{2j_2}$. Then, for $i = 1, 2$, the first variations

$$\overline{u}_i(x) = \frac{\partial u_i(Y_i; x)}{\partial Y_{i,j_i}} \cdot V, \quad \overline{\phi}_i(x) = \frac{\partial \phi_i(Y_i; x)}{\partial Y_{i,j_i}} \cdot V \tag{5.28}$$

exist and satisfy: there exist $C, \gamma > 0$, independent of R, such that for all $|y| \leq R$

$$\sum_{|\alpha| \leq 2} \big(|\partial^\alpha(\overline{u}_1 - \overline{u}_2)(y)| + |\partial^\alpha(\overline{\phi}_1 - \overline{\phi}_2)(y)|\big) \leq C|V|e^{-\gamma(|y - Y_{1j_1}| + R - |y|)}. \tag{5.29}$$

We remark that the proof of Lemma 5.7 requires Corollary 5.10, which is shown in the next subsection. For this reason, we postpone the proof of Lemma 5.7 to page 139.

It is also straightforward to adapt Lemma 5.6 to linearise the TFW Yukawa equations.

As $m_h \in \mathcal{Y}_{L^2}(M', \omega')$ for all $h \in [0, 1]$, by Proposition 2.5 for all $a > 0$ there exist corresponding Yukawa ground states $(u_a, \phi_a) = (u_{a,0}, \phi_{a,0})$ and $(u_{a,h}, \phi_{a,h})$.

Lemma 5.8. *Let $a_0 > 0$, $Y \in \mathcal{Y}_{L^2}(M, \omega)$ and let $m = m_Y \in \mathcal{M}_{L^2}(M, \omega)$.*

Also, let $k \in \mathbb{N}$, $V \in \mathbb{R}^3$ and $h_0 = (1+|V|)^{-1}$. For $h \in [0, h_0]$ define

$$m_h(x) = m(x) + \eta(x - Y_k - hV) - \eta(x - Y_k),$$

1. *For all $0 < a \leq a_0$ and $h \in [0, h_0]$ there exists a unique Yukawa ground state $(u_{a,h}, \phi_{a,h})$ corresponding to m_h. There exist $C = C(a_0, M', \omega')$, $\gamma_0 = \gamma_0(a_0, M', \omega') > 0$, independent of a, h and $|V|$, such that for all $0 < a \leq a_0$ and $h \in [0, h_0]$*

$$\begin{aligned} \sum_{|\alpha| \leq 2} \big(|\partial^\alpha (u_{a,h} - u_a)(x)| + |\partial^\alpha (\phi_{a,h} - \phi_a)(x)| \big) + |(m_h - m)(x)| & \\ \leq Ch|V|e^{-\gamma|x - Y_k|}, & \quad (5.30) \\ \|u_{a,h} - u_a\|_{H^4(\mathbb{R}^3)} + \|\phi_{a,h} - \phi_a\|_{H^2(\mathbb{R}^3)} \leq C\|m_h - m\|_{L^2(\mathbb{R}^3)} & \\ \leq Ch|V|. & \quad (5.31) \end{aligned}$$

2. *For all $0 < a \leq a_0$, there exist $\overline{u}_a \in H^4(\mathbb{R}^3), \overline{\phi}_a \in H^2(\mathbb{R}^3)$ and $\overline{m} \in C_c^\infty(\mathbb{R}^3)$ such that $\frac{u_{a,h} - u_a}{h}, \frac{\phi_{a,h} - \phi_a}{h}$ converge to $\overline{u}_a, \overline{\phi}_a$ respectively, weakly in $H^4(\mathbb{R}^3)$ and $H^2(\mathbb{R}^3)$, strongly in $H^3(B_R(0))$ and $H^1(B_R(0))$ for all $R > 0$ and pointwise almost everywhere, along with their derivatives. In addition, $\frac{m_h - m}{h}$ converges pointwise to $\overline{m}$.*

   The pair $(\overline{u}_a, \overline{\phi}_a)$ is the unique solution to the linearised TFW Yukawa equations

$$- \Delta \overline{u}_a + \left(\frac{35}{9} u_a^{4/3} - \phi_a \right) \overline{u}_a - u_a \overline{\phi}_a = 0, \quad (5.32a)$$

$$- \Delta \overline{\phi}_a + a^2 \overline{\phi}_a = 4\pi \left(\overline{m} - 2 u_a \overline{u}_a \right). \quad (5.32b)$$

3. *Moreover, for all $0 < a \leq a_0$, $\overline{u}_a, \overline{\phi}_a$ and $\overline{m}$ satisfy*

$$\sum_{|\alpha| \leq 2} \big(|\partial^\alpha \overline{u}_a(x)| + |\partial^\alpha \overline{\phi}_a(x)| \big) + |\overline{m}(x)| \leq C|V|e^{-\gamma|x - Y_k|}, \quad (5.33)$$

$$\|\overline{u}_a\|_{H^4(\mathbb{R}^3)} + \|\overline{\phi}_a\|_{H^2(\mathbb{R}^3)} \leq C\|\overline{m}\|_{L^2(\mathbb{R}^3)}, \quad (5.34)$$

   where the constants $C = C(a_0, M', \omega')$, $\gamma = \gamma(a_0, M', \omega') > 0$ are independent of a and $|V|$.

Proof of Lemma 5.6. By Lemma 5.3 and Propositions 2.1, 2.2, for $h \in [0, h_0]$

the ground state (u_h, ϕ_h) satisfies

$$\|u_h\|_{H^4_{\text{unif}}(\mathbb{R}^3)} + \|\phi_h\|_{H^2_{\text{unif}}(\mathbb{R}^3)} \le C(M'), \tag{5.35}$$
$$\inf_{x\in\mathbb{R}^3} u_h(x) \ge c_{M',\omega'} > 0, \tag{5.36}$$

independently of h. From (5.17), it follows that

$$\begin{aligned}|(m_h - m)(x)| &= |\eta(x - Y_k - hV) - \eta(x - Y_k)| \\ &= h|V| \left|\int_0^1 \nabla\eta(x - Y_k - thV)\ \mathrm{d}t\right| \\ &\le h|V| \int_0^1 |\nabla\eta(x - Y_k - thV)|\ \mathrm{d}t, \end{aligned} \tag{5.37}$$

and moreover

$$\|m_h - m\|_{L^\infty(\mathbb{R}^3)} \le h|V|\|\nabla\eta\|_{L^\infty(\mathbb{R}^3)}. \tag{5.38}$$

For all $h \in [0, h_0]$, $\operatorname{spt}(m_h - m) \subset B_{R_0+1}(Y_k)$, so by Corollary 3.9 and (5.37)–(5.38), there exist C, $\gamma_0 > 0$ such that

$$\sum_{|\alpha|\le 2} |\partial^\alpha(u_h - u)(x)| + |(\phi_h - \phi)(x)| + |(m_h - m)(x)| \le Ch|V|e^{-\gamma_0|x-Y_k|}, \tag{5.39}$$

and (5.23) holds

$$\|u_h - u\|_{H^4(\mathbb{R}^3)} + \|\phi_h - \phi\|_{H^2(\mathbb{R}^3)} \le C\|m_h - m\|_{L^2(\mathbb{R}^3)} \le Ch|V|.$$

Due to the uniform estimates (5.35)–(5.36) and (5.37), the constants appearing on the right-hand side are independent of h and $|V|$.

It remains to show the additional estimate

$$\sum_{|\alpha|\le 2} |\partial^\alpha(\phi_h - \phi)(x)| \le Ch|V|e^{-\gamma_0|x-Y_k|}. \tag{5.40}$$

Recall that as $\operatorname{spt}(\eta) \subset B_{R_0}(0)$, $\operatorname{spt}(m_h - m) \subset B_{R_0+1}(Y_k)$ for all $h \in (0, h_0]$. Applying the triangle inequality, for $x \in B^{\mathrm{c}}_{R_0+3}(Y_k)$ it follows that

$B_2(x) \subset B^{\mathrm{c}}_{R_0+1}(Y_k)$. Consequently, for $x \in B^{\mathrm{c}}_{R_0+3}(Y_k)$

$$\|m_h - m\|_{C^{0,1/2}(B_2(x))} = 0. \tag{5.41}$$

Alternatively, for $x \in B_{R_0+3}(Y_k)$, by (5.37) it follows that

$$\begin{aligned}\|m_h - m\|_{C^{0,1/2}(B_2(x))} &\leq h|V| \left\| \int_0^1 \nabla\eta(\cdot - Y_k - thV)\,\mathrm{d}t \right\|_{C^{0,1/2}(B_2(x))} \\ &\leq Ch|V| \left(\|\nabla\eta\|_{L^\infty(\mathbb{R}^3)} + \|\nabla^2\eta\|_{L^\infty(\mathbb{R}^3)} \right), \end{aligned} \tag{5.42}$$

where the final constant is independent of $x \in \mathbb{R}^3$. By (5.41)–(5.42) we deduce that $x \mapsto \|m_h - m_0\|_{C^{0,1/2}(B_2(x))}$ is a bounded function with support in $B_{R_0+3}(Y_k)$, hence there exists $C > 0$ such that

$$\|m_h - m\|_{C^{0,1/2}(B_2(x))} \leq Ch|V|e^{-\gamma_0|x-Y_k|}. \tag{5.43}$$

Then, using that $\phi_h - \phi$ solves

$$-\Delta(\phi_h - \phi) = 4\pi(m_h - m - u_h^2 + u^2),$$

we apply the Schauder estimates [35, Theorem 10.2.1, Lemma 10.1.1] together with (5.39) and (5.43) to estimate

$$\begin{aligned}&\|\phi_h - \phi\|_{C^{2,1/2}(B_1(x))} \\ &\qquad \leq C\left(\|m_h - m - u_h^2 + u^2\|_{C^{0,1/2}(B_2(x))} + \|\phi_h - \phi\|_{L^2(B_2(x))} \right), \\ &\qquad \leq C\left(\|m_h - m\|_{C^{0,1/2}(B_2(x))} + \|u_h^2 - u^2\|_{C^{0,1/2}(B_2(x))} \right) \\ &\qquad\qquad + C\|\phi_h - \phi\|_{L^2(B_2(x))}, \\ &\qquad \leq C\left(\|(u_h + u)(u_h - u)\|_{C^{0,1/2}(B_2(x))} + h|V|e^{-\gamma_0|x-Y_k|} \right), \\ &\qquad \leq C\left(\|u_h + u\|_{C^{0,1/2}(B_2(x))}\|u_h - u\|_{C^{0,1/2}(B_2(x))} + h|V|e^{-\gamma_0|x-Y_k|} \right). \end{aligned} \tag{5.44}$$

Applying the Sobolev embedding $H^2(B_2(x)) \hookrightarrow C^{0,1/2}(B_2(x))$ [24, Section

5.6.3, Theorem 6], and using (5.36), it follows that

$$\begin{aligned}\|u_h+u\|_{C^{0,1/2}(B_2(x))} &\le C\|u_h+u\|_{H^2(B_2(x))}\\ &\le C\left(\|u_h\|_{H^2_{\text{unif}}(\mathbb{R}^3)}+\|u\|_{H^2_{\text{unif}}(\mathbb{R}^3)}\right)\le C_0. \qquad (5.45)\end{aligned}$$

Applying (5.45) and (5.39) to (5.44), we obtain the desired estimate (5.40): for any multi-index α satisfying $|\alpha|\le 2$

$$\begin{aligned}|\partial^\alpha(\phi_h-\phi)(x)| &\le \|\phi_h-\phi\|_{C^{2,1/2}(B_1(x))}\\ &\le C\left(\|u_h+u\|_{C^{0,1/2}(B_2(x))}\|u_h-u\|_{C^{0,1/2}(B_2(x))}+h|V|e^{-\gamma_0|x-Y_k|}\right)\\ &\le C\left(C_0\|u_h-u\|_{H^2(B_2(x))}+h|V|e^{-\gamma_0|x-Y_k|}\right)\le Ch|V|e^{-\gamma_0|x-Y_k|}.\end{aligned}$$

We will show next that there exist $\overline{u}\in H^4(\mathbb{R}^3), \overline{\phi}\in H^2(\mathbb{R}^3)$ such that $\frac{u_h-u}{h}, \frac{\phi_h-\phi}{h}$ converge to $\overline{u}, \overline{\phi}$ respectively, weakly in $H^4(\mathbb{R}^3)$ and $H^2(\mathbb{R}^3)$, strongly in $H^3(B_R(0))$ and $H^1(B_R(0))$ for all $R>0$ and pointwise almost everywhere, along with their derivatives as $h\to 0$.

First consider any decreasing sequence $h_n\to 0$, then there exists a subsequence (still denoted by h_n) such that $\frac{u_{h_n}-u}{h_n}, \frac{\phi_{h_n}-\phi}{h_n}$ converge to $\overline{u}\in H^4(\mathbb{R}^3), \overline{\phi}\in H^2(\mathbb{R}^3)$ respectively, weakly in $H^4(\mathbb{R}^3)$ and $H^2(\mathbb{R}^3)$, strongly in $H^3(B_R(0))$ and $H^1(B_R(0))$ for all $R>0$ and pointwise almost everywhere, along with their derivatives. In addition, it follows that $(\overline{u}, \overline{\phi})$ satisfy (5.25)–(5.26).

We now verify that the limiting functions are independent of the choice of sequence. First, observe that by passing to the limit as $h_n\to 0$ in the equations

$$\begin{aligned}&-\Delta\left(\frac{u_{h_n}-u}{h_n}\right)+\frac{5}{3}\frac{u_{h_n}^{7/3}-u^{7/3}}{h_n}-\frac{\phi_{h_n}u_{h_n}-\phi u}{h_n}=0,\\ &-\Delta\left(\frac{\phi_{h_n}-\phi}{h_n}\right)=4\pi\left(\frac{m_{h_n}-m}{h_n}-\frac{u_{h_n}^2-u^2}{h_n}\right),\end{aligned}$$

it follows that $(\overline{u}, \overline{\phi})$ solve the linearised TFW equations (5.24) pointwise,

$$\begin{aligned}
&-\Delta \overline{u} + \left(\frac{35}{9}u^{4/3} - \phi\right)\overline{u} - u\overline{\phi} = 0, \\
&-\Delta \overline{\phi} = 4\pi\left(\overline{m} - 2u\overline{u}\right), \\
\text{where} \quad &\overline{m}(x) = \lim_{h_n \to 0} \frac{(m_{h_n} - m)(x)}{h_n} = -\nabla\eta(x - Y_k)\cdot V.
\end{aligned}$$

Clearly $\overline{m}$ is independent of the sequence h_n. Applying [8, Corollary 2.3], it follows that the $(\overline{u}, \overline{\phi})$ is the unique solution to the linearised system (5.24), hence is independent of the sequence (h_n). It then follows that $\frac{u_h - u}{h}, \frac{\phi_h - \phi}{h}$ converge to $\overline{u}, \overline{\phi}$ as $h \to 0$ as stated above. □

Proof of Lemma 5.8. The first step is to show the uniqueness of the linearised Yukawa solution $(\overline{u}_a, \overline{\phi}_a)$ to (5.32). Let $0 < a \leq a_0$ and suppose that $(w, \psi) \in H^1(\mathbb{R}^3) \times H^1(\mathbb{R}^3)$ solves

$$-\Delta w + \left(\frac{35}{9}u_a^{4/3} - \phi_a\right)w - u_a\psi = 0, \tag{5.46a}$$

$$-\Delta\psi + a^2\psi = -8\pi u_a\psi. \tag{5.46b}$$

Testing (5.46a) with w yields

$$\int_{\mathbb{R}^3} |\nabla w|^2 + \int_{\mathbb{R}^3}\left(\frac{35}{9}u_a^{4/3} - \phi_a\right)w^2 = \int_{\mathbb{R}^3} u_a w\psi.$$

Then as $u_a > 0$, by Lemma 2.8 $L_a = -\Delta + \frac{35}{9}u_a^{4/3} - \phi_a$ is a non-negative operator. In addition, by Proposition 2.6 $\inf u_a \geq c_{a_0, M', \omega'} > 0$, hence there exists $c_0 > 0$ such that

$$\begin{aligned}
c_0 \int_{\mathbb{R}^3} w^2 \leq \frac{10}{9}\int_{\mathbb{R}^3} u_a^{4/3}w^2 &\leq \langle w, L_a w\rangle + \frac{10}{9}\int_{\mathbb{R}^3} u_a^{4/3}w^2 \\
&= \int_{\mathbb{R}^3} |\nabla w|^2 + \int_{\mathbb{R}^3}\left(\frac{35}{9}u_a^{4/3} - \phi_a\right)w^2 = \int_{\mathbb{R}^3} u_a w\psi.
\end{aligned} \tag{5.47}$$

Then testing (5.46b) with $\frac{1}{8\pi}\psi$ gives

$$\frac{1}{8\pi}\left(\int_{\mathbb{R}^3} |\nabla\psi|^2 + a^2\int_{\mathbb{R}^3}\psi^2\right) = -\int_{\mathbb{R}^3} u_a w\psi, \tag{5.48}$$

and adding (5.47)–(5.48) yields

$$0 \leq c_0 \int_{\mathbb{R}^3} w^2 + \frac{1}{8\pi} \left(\int_{\mathbb{R}^3} |\nabla \psi|^2 + a^2 \int_{\mathbb{R}^3} \psi^2 \right) \leq 0,$$

hence $w = \psi = 0$ almost everywhere, so (5.32) has a unique solution in $H^1(\mathbb{R}^3) \times H^1(\mathbb{R}^3)$. Now, Proposition 2.4 and Proposition 2.14 imply that for $0 < a \leq a_0$ and $h \in [0, h_0]$ the ground state $(u_{a,h}, \phi_{a,h})$ satisfies

$$\begin{aligned} &\|u_{a,h}\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\phi_{a,h}\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(a_0, M'), \\ &\inf_{x \in \mathbb{R}^3} u_{a,h}(x) \geq c_{a_0, M', \omega'} > 0, \end{aligned}$$

independently of a, h and $|V|$. Then following the proof of Lemma 5.6, for all $0 < a \leq a_0$ and $h \in [0, h_0]$, the estimates (5.30)–(5.31) hold. In addition, there exist $\overline{u}_a \in H^4(\mathbb{R}^3)$ and $\overline{\phi}_a \in H^2(\mathbb{R}^3)$ such that along a subsequence h_n (which may depend on a) such that $\frac{u_{a,h_n} - u_a}{h_n}$, $\frac{\phi_{a,h_n} - \phi_a}{h_n}$ converge to $\overline{u}_a \in H^4(\mathbb{R}^3)$ and $\overline{\phi}_a \in H^2(\mathbb{R}^3)$ respectively, weakly in $H^4(\mathbb{R}^3)$ and $H^2(\mathbb{R}^3)$, strongly in $H^3(B_R(0))$ and $H^1(B_R(0))$ for all $R > 0$ and pointwise almost everywhere, along with their derivatives. In addition, it follows that $(\overline{u}_a, \overline{\phi}_a)$ satisfy (5.33)–(5.34).

To verify that $(\overline{u}_a, \overline{\phi}_a)$ are independent of the sequence chosen, passing to the limit in the equations

$$\begin{aligned} &-\Delta \left(\frac{u_{a,h_n} - u_a}{h_n} \right) + \frac{5}{3} \frac{u_{a,h_n}^{7/3} - u_a^{7/3}}{h_n} - \frac{\phi_{a,h_n} u_{a,h_n} - \phi_a u_a}{h_n} = 0, \\ &-\Delta \left(\frac{\phi_{a,h_n} - \phi_a}{h_n} \right) + a^2 \left(\frac{\phi_{a,h_n} - \phi_a}{h_n} \right) = 4\pi \left(\frac{m_{h_n} - m}{h_n} - \frac{u_{a,h_n}^2 - u_a^2}{h_n} \right), \end{aligned}$$

gives that $(\overline{u}_a, \overline{\phi}_a)$ solve the linearised Yukawa equations (5.32) pointwise,

$$\begin{aligned} &-\Delta \overline{u}_a + \left(\frac{35}{9} u_a^{4/3} - \phi_a \right) \overline{u}_a - u_a \overline{\phi}_a = 0, \\ &-\Delta \overline{\phi}_a + a^2 \overline{\phi}_a = 4\pi \left(\overline{m} - 2 u_a \overline{u}_a \right), \\ \text{where} \quad &\overline{m}(x) = \lim_{h_n \to 0} \frac{(m_{h_n} - m)(x)}{h_n} = -\nabla \eta(x - Y_k) \cdot V. \end{aligned}$$

Clearly $\overline{m}$ is independent of the sequence h_n, so as $(\overline{u}_a, \overline{\phi}_a)$ is the unique solution to the linearised Yukawa system (5.32), it is independent of the sequence (h_n). It then follows that $\frac{u_{a,h}-u_a}{h}, \frac{\phi_{a,h}-\phi_a}{h}$ converge to $\overline{u}_a, \overline{\phi}_a$ as $h \to 0$ as stated above. $\square$

5.5 Higher variations of the TFW equations

We introduce a definition for higher derivatives of a function with respect to nuclear perturbations. We remark that this notation differs from the notation used to describe the linearised TFW equations (5.24).

Definition 2. *Consider a function $f : \mathcal{Y}_{L^2}(M', \omega') \times \mathbb{R}^3 \to \mathbb{R}$. For $k \in \mathbb{N}$, $Y \in \mathcal{Y}_{L^2}(M', \omega'), x \in \mathbb{R}^3$ and $\mathbf{V} \in (\mathbb{R}^3)^k, \mathbf{n} \in \mathbb{N}^k$ and define the derivative*

$$f_{\mathbf{V},\mathbf{n}}(Y;x) = \left\langle \frac{\partial^k f(Y;x)}{\partial Y_{n_1} \cdots \partial Y_{n_k}}, \mathbf{V} \right\rangle, \tag{5.49}$$

whenever the right-hand side is well-defined. The derivative $\frac{\partial^k f(Y;x)}{\partial Y_{n_1} \cdots \partial Y_{n_k}} \in \mathbb{R}^{3^k}$ acts as a k-linear function that maps $(\mathbb{R}^3)^k$ to $\mathbb{R}$. $\square$

Remark 15. We give a brief justification of the notation introduced in Definition 2. As each $Y_j \in \mathbb{R}^3$, for $j \in \mathbb{N}$, it follows that derivatives of the form $\frac{\partial^k f(Y;x)}{\partial Y_{n_1} \cdots \partial Y_{n_k}} \in \mathbb{R}^{3^k}$. Consequently, treating each component of the k-th variation of the TFW equations separately would require us to consider the existence, uniqueness and locality of $\mathbb{R}^{3^k}$ distinct coupled PDE systems in total. Instead, by using the notation introduced in (5.49), the k-th variation of the TFW equations can be described using a single coupled PDE system.

Remark 16. Recall the definition (5.1)

$$m_Y(x) = \sum_{j \in \mathbb{N}} \eta(x - Y_j),$$

where $\eta \in C_c^\infty(\mathbb{R}^3)$. It follows that for any $Y \in \mathcal{Y}_{L^2}(M, \omega)$, $k \in \mathbb{N}$ and $\mathbf{V} \in (\mathbb{R}^3)^k, \mathbf{n} \in \mathbb{N}^k$, for $m = m_Y = m(Y; \cdot)$, the derivative $m_{\mathbf{V},\mathbf{n}}$ exists and

$$m_{\mathbf{V},\mathbf{n}}(Y;x) = (-1)^k \left\langle \nabla^k \eta(x - Y_{n_1}) \prod_{i=2}^{k} \delta_{n_1}(n_i), \mathbf{V} \right\rangle, \tag{5.50}$$

In particular, if $n_i \neq n_1$ for some $2 \leq i \leq k$, then $m_{\mathbf{V},\mathbf{n}} = 0$. As $\eta \in C_{\mathrm{c}}^{\infty}(\mathbb{R}^3)$ there exists $C = C_k, \gamma > 0$ such that

$$|m_{\mathbf{V},\mathbf{n}}(Y;x)| \leq C \prod_{i=1}^{k} |V_i| e^{-\gamma |x - Y_{n_i}|} \tag{5.51}$$

□

Theorem 5.9. *Let $Y \in \mathcal{Y}_{L^2}(M,\omega)$, $m = m_Y \in \mathcal{M}_{L^2}(M,\omega)$ and (u_0, ϕ_0) denote the corresponding ground state. Further, let $k \in \mathbb{N}$ and $\mathbf{V} \in (\mathbb{R}^3)^k$ and $\mathbf{n} \in \mathbb{N}^k$. Then, there exists a unique solution $(u_{\mathbf{V},\mathbf{n}}, \phi_{\mathbf{V},\mathbf{n}})$ to the k-th variation of the TFW equations*

$$\begin{aligned} -\Delta u_{\mathbf{V},\mathbf{n}} + \left(\frac{35}{9} u_0^{4/3} - \phi_0 \right) u_{\mathbf{V},\mathbf{n}} - u_0 \phi_{\mathbf{V},\mathbf{n}} &= R^{(1)}_{k,\mathbf{V},\mathbf{n}}, \\ -\Delta \phi_{\mathbf{V},\mathbf{n}} &= 4\pi \left(m_{\mathbf{V},\mathbf{n}} - 2 u_0 u_{\mathbf{V},\mathbf{n}} \right) + R^{(2)}_{k,\mathbf{V},\mathbf{n}}, \end{aligned}$$

where $u_{\mathbf{V},\mathbf{n}} \in H^4(\mathbb{R}^3), \phi_{\mathbf{V},\mathbf{n}} \in H^2(\mathbb{R}^3), m_{\mathbf{V},\mathbf{n}} \in C_{\mathrm{c}}^{\infty}(\mathbb{R}^3)$ and also $R^{(1)}_{k,\mathbf{V},\mathbf{n}}, R^{(2)}_{k,\mathbf{V},\mathbf{n}} \in L^1(\mathbb{R}^3)$.

Moreover, there exists $C = C_C(k, M', \omega')$, $\gamma_0 = \gamma_0(M', \omega') > 0$ such that

$$\sum_{|\alpha| \leq 2} \left(|\partial^\alpha u_{\mathbf{V},\mathbf{n}}(x)| + |\partial^\alpha \phi_{\mathbf{V},\mathbf{n}}(x)| \right) \leq C \prod_{i=1}^{k} |V_i| e^{-\gamma_0 |x - Y_{n_i}|}, \tag{5.53}$$

$$|m_{\mathbf{V},\mathbf{n}}(x)| + |R^{(1)}_{k,\mathbf{V},\mathbf{n}}(x)| + |R^{(2)}_{k,\mathbf{V},\mathbf{n}}(x)| \leq C \prod_{i=1}^{k} |V_i| e^{-\gamma_0 |x - Y_{n_i}|}, \tag{5.54}$$

$$\begin{aligned} &\|u_{\mathbf{V},\mathbf{n}}\|_{H^4(\mathbb{R}^3)} + \|\phi_{\mathbf{V},\mathbf{n}}\|_{H^2(\mathbb{R}^3)} \\ &\quad \leq C \Big(\|m_{\mathbf{V},\mathbf{n}}\|_{L^2(\mathbb{R}^3)} + \|R^{(1)}_{k,\mathbf{V},\mathbf{n}}\|_{L^2(\mathbb{R}^3)} + \|R^{(2)}_{k,\mathbf{V},\mathbf{n}}\|_{L^2(\mathbb{R}^3)} \Big). \end{aligned} \tag{5.55}$$

Remark 17. The residual functions $R^{(1)}_{k,\mathbf{V},\mathbf{n}}, R^{(1)}_{k,\mathbf{V},\mathbf{n}}$ are defined inductively by the following relations. When $k = 1$, $R^{(1)}_{1,\mathbf{V},\mathbf{n}} = R^{(2)}_{1,\mathbf{V},\mathbf{n}} = 0$. For $\mathbf{V}' \in (\mathbb{R}^3)^{k+1}$ and $\mathbf{n}' \in \mathbb{N}^{k+1}$, let $\mathbf{V} \in (\mathbb{R}^3)^k, \mathbf{n} \in \mathbb{N}^k$ satisfy $\mathbf{V}' = (\mathbf{V}', V_{k+1}), \mathbf{n}' = (\mathbf{n}', n_{k+1})$.

Then given $R^{(1)}_{k,\mathbf{V},\mathbf{n}}, R^{(2)}_{k,\mathbf{V},\mathbf{n}}$, define

$$
\begin{aligned}
R^{(1)}_{k+1,\mathbf{V}',\mathbf{n}'}(Y;x) &= \frac{\partial R^{(1)}_{k,\mathbf{V},\mathbf{n}}(Y;x)}{\partial Y_{n_{k+1}}} \cdot V_{k+1} \\
&\quad + \left(\phi_{V_{k+1},n_{k+1}} - \frac{120}{27} u_0^{1/3} u_{V_{k+1},n_{k+1}} \right) u_{\mathbf{V},\mathbf{n}} + u_{V_{k+1},n_{k+1}} \phi_{\mathbf{V},\mathbf{n}}, \\
R^{(2)}_{k+1,\mathbf{V}',\mathbf{n}'}(Y;x) &= \frac{\partial R^{(2)}_{k,\mathbf{V},\mathbf{n}}(Y;x)}{\partial Y_{n_{k+1}}} \cdot V_{k+1} - 8\pi u_{V_{k+1},n_{k+1}} u_{\mathbf{V},\mathbf{n}}.
\end{aligned}
$$

It follows that $R^{(1)}_{k,\mathbf{V},\mathbf{n}}, R^{(2)}_{k,\mathbf{V},\mathbf{n}}$ are a finite combination of products and sums of the first $k-1$ variations of the TFW equations, hence are differentiable with respect to nuclear perturbations. $\square$

In order to prove Theorem 5.9, we first show the following result, which generalises (3.8) from Theorem 3.1 to show that every variation of the TFW equations satisfies a pointwise stability estimate.

Corollary 5.10. *Let $m \in \mathcal{M}_{L^2}(M,\omega)$ and let (u_0,ϕ_0) denote the corresponding ground state. Further, suppose there exist $w,\psi : \mathbb{R}^3 \to \mathbb{R}$ satisfying*

$$
\|w\|_{H^4_{\mathrm{unif}}(\mathbb{R}^3)} + \|\psi\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq M',
$$

that also solve the following coupled system of equations

$$
\begin{aligned}
&-\Delta w + \left(\frac{35}{9} u_0^{4/3} - \phi_0 \right) w - u_0 \psi = T_1, \\
&-\Delta \psi = -8\pi u_0 w + T_2,
\end{aligned}
$$

where $T_1, T_2 \in L^2(\mathbb{R}^3)$. Then, there exist $C = C(M,M',\omega) > 0$ and $\gamma = \gamma(M,M',\omega) > 0$ such that for all $y \in \mathbb{R}^3$

$$
\begin{aligned}
&\sum_{|\alpha|\leq 2} \left(|\partial^\alpha w(y)| + |\partial^\alpha \psi(y)| \right) \\
&\qquad \leq C \left(\int_{\mathbb{R}^3} \left(|(T_1(x)|^2 + |T_2(x)|^2 \right) e^{-2\gamma|x-y|} \, \mathrm{d}x \right)^{1/2}, \qquad (5.57) \\
&\|w\|_{H^4(\mathbb{R}^3)} + \|\psi\|_{H^2(\mathbb{R}^3)} \leq C \left(\|T_1\|_{L^2(\mathbb{R}^3)} + \|T_2\|_{L^2(\mathbb{R}^3)} \right). \qquad (5.58)
\end{aligned}
$$

We first prove Theorem 5.9 assuming that Corollary 5.10 holds, then verify this assertion.

Proof of Theorem 5.9. We argue by induction and follow the argument used to prove Lemma 5.6. Observe that the case $k = 1$ has been shown in Lemma 5.6, so suppose (5.52)–(5.54) hold for all k' variation of the TFW equations, where $1 \leq k' \leq k$. For any $\mathbf{V}' \in (\mathbb{R}^3)^{k+1}, \mathbf{n}' \in \mathbb{N}^{k+1}$, let $\mathbf{V} \in (\mathbb{R}^3)^k, \mathbf{n} \in \mathbb{N}^k$ satisfy $\mathbf{V}' = (\mathbf{V}, V_{k+1}), \mathbf{n}' = (\mathbf{n}, n_{k+1})$. In addition, let $Y \in \mathcal{Y}_{L^2}(M, \omega)$, then let $h_0 = (1 + |V_{k+1}|)^{-1}$ and for $h \in [0, h_0]$, define

$$Y^h = \{\, Y_j + \delta_{n_{k+1}}(j) h V_{k+1} \,|\, j \in \mathbb{N} \,\}.$$

Using (5.50), for $h \in [0, h_0]$ define $m_{h,k} = m_{\mathbf{V},\mathbf{n}}(Y^h; \cdot)$ and denote the corresponding k-th order variations by $(u_{h,k}, \phi_{h,k})$, which solve

$$\begin{aligned}
-\Delta u_{h,k} + \left(\frac{35}{9} u_h^{4/3} - \phi_h \right) u_{h,k} - u_h \phi_{h,k} &= R^{(1)}_{h,k}, \\
-\Delta \phi_{h,k} = 4\pi \left(m_{h,k} - 2 u_h u_{h,k} \right) &+ R^{(2)}_{h,k},
\end{aligned}$$

where $u_h = u_0(Y^h; \cdot), \phi_h = \phi_0(Y^h; \cdot)$ and for $i = 1, 2$ $R^{(i)}_{h,k} = R^{(i)}_{k,\mathbf{V},\mathbf{n}}(Y^h; \cdot)$. As (5.53) is satisfied, there exists $\gamma_0 > 0$ such that

$$|u_{h,k}(x)| + |\phi_{h,k}(x)| \leq C \prod_{i=1}^{k} |V_i| e^{-\gamma_0 |x - Y_{n_i}|}, \tag{5.60}$$

We now show a stability for the k-th variation of the TFW equations (5.52), which follows as a direct consequence of the stability of the linearised TFW equations.

Define the differences $w_{h,k} = u_{h,k} - u_{0,k}, \psi_{h,k} = \phi_{h,k} - \phi_{0,k}$ and for $i = 1, 2$, $S^{(i)}_{h,k} = R^{(i)}_{h,k} - R^{(i)}_{0,k}$. The difference $(w_{h,k}, \psi_{h,k})$ solves

$$\begin{aligned}
&- \Delta w_{h,k} + \left(\frac{35}{9} u_0^{4/3} - \phi_0 \right) w_{h,k} - u_0 \psi_{h,k} \\
&\qquad = (u_h - u_0)\phi_{h,k} - \left(\frac{35}{9} (u_h^{4/3} - u_0^{4/3}) - (\phi_h - \phi_0) \right) u_{h,k} + S^{(1)}_{h,k}, \qquad (5.61a) \\
&- \Delta \psi_{h,k} = 4\pi \left(m_{h,k} - m_{0,k} - 2 u_0 w_{h,k} \right) - 8\pi (u_h - u_0) u_{h,k} + S^{(2)}_{h,k}. \qquad (5.61b)
\end{aligned}$$

By (5.22) of Lemma 5.6, there exists $\gamma_1 > 0$ such that

$$\sum_{|\alpha|\le 2} \left(|\partial^\alpha (u_h - u_0)(x)| + |\partial^\alpha (\phi_h - \phi_0)(x)|\right) \le Ch|V_{n_{k+1}}|e^{-\gamma_1|x-Y_{n_{k+1}}|}.$$

In addition, applying (5.51), there exists $\gamma_2 > 0$ such that

$$\begin{aligned} |(m_h - m_0)(x)| = |m_{\mathbf{V},\mathbf{n}}(Y^h; x) - m_{\mathbf{V},\mathbf{n}}(Y; x)| &\le \int_0^1 \left| \frac{\partial m_{\mathbf{V},\mathbf{n}}(Y^{th}; x)}{\partial Y_{n_{k+1}}} \cdot V_{n_{k+1}} \right| \,\mathrm{d}t \\ &= \int_0^1 |m_{\mathbf{V}',\mathbf{n}'}(Y^{th}; x)| \,\mathrm{d}t \le C \prod_{i=1}^{k+1} |V_i| e^{-\gamma_2|x-Y_{n_i}|}. \end{aligned} \tag{5.62}$$

It follows from Remark 17 that the difference functions $S^{(i)}_{h,k}$ are functions of the first $k-1$ variations of the TFW equations, hence are differentiable with respect to nuclear perturbations. For $i = 1, 2$, applying (5.53) yields

$$\begin{aligned} \left|S^{(i)}_{h,k}(x)\right| = \left|R^{(i)}_{\mathbf{V},\mathbf{n}}(Y^h; x) - R^{(i)}_{\mathbf{V},\mathbf{n}}(Y; x)\right| &\le \int_0^1 \left| \frac{\partial R^{(i)}_{\mathbf{V},\mathbf{n}}(Y^{th}; x)}{\partial Y_{n_{k+1}}} \cdot hV_{n_{k+1}} \right| \,\mathrm{d}t \\ &= h\int_0^1 \left|R^{(i)}_{\mathbf{V}',\mathbf{n}'}(Y^{th}; x)\right| \,\mathrm{d}t \le Ch \prod_{i=1}^{k+1} |V_i| e^{-\gamma_0|x-Y_{n_i}|}. \end{aligned} \tag{5.63}$$

It follows from (5.62)–(5.63) that the system of equations (5.61a)–(5.61b) can be written as

$$-\Delta w_{h,k} + \left(\frac{35}{9} u_0^{4/3} - \phi_0\right) w_{h,k} - u_0 \psi_{h,k} = T^{(1)}_{h,k}, \tag{5.64a}$$

$$-\Delta \psi_{h,k} = -8\pi u_0 w_{h,k} + T^{(2)}_{h,k}, \tag{5.64b}$$

where $T^{(1)}_{h,k}, T^{(2)}_{h,k} \in L^2(\mathbb{R}^3)$ and

$$\left\|T^{(1)}_{h,k}\right\|_{L^2(\mathbb{R}^3)} + \left\|T^{(2)}_{h,k}\right\|_{L^2(\mathbb{R}^3)} \le Ch. \tag{5.65}$$

Moreover, collecting the estimates (5.60)–(5.63), we deduce

$$
\begin{aligned}
\left|T_{h,k}^{(1)}(x)\right| + \left|T_{h,k}^{(2)}(x)\right| &\le \left(|(u_h - u_0)(x)| + |(\phi_h - \phi_0)(x)|\right)\left(|u_{h,k}(x)| + |\phi_{h,k}(x)|\right) \\
&\qquad + |(m_{h,k} - m_{0,k})(x)| + \left|S_{h,k}^{(1)}(x)\right| + \left|S_{h,k}^{(2)}(x)\right| \\
&\le Ch|V_{k+1}|e^{-\gamma_1|x-Y_{n_{k+1}}|}\prod_{i=1}^{k}|V_i|e^{-\gamma_0|x-Y_{n_i}|} \\
&\qquad + Ch\prod_{i=1}^{k+1}|V_i|\left(e^{-\gamma_0|x-Y_{n_i}|} + e^{-\gamma_2|x-Y_{n_i}|}\right) \\
&\le Ch\prod_{i=1}^{k+1}|V_i|e^{-\widetilde{\gamma}|x-Y_{n_i}|},
\end{aligned} \tag{5.66}
$$

where $\widetilde{\gamma} = \min_{0\le i\le 2}\gamma_i > 0$. Applying Corollary 5.10, we deduce from (5.65) that

$$
\|w_{h,k}\|_{H^4(\mathbb{R}^3)} + \|\psi_{h,k}\|_{H^2(\mathbb{R}^3)} \le C\left(\left\|T_{h,k}^{(1)}\right\|_{L^2(\mathbb{R}^3)} + \left\|T_{h,k}^{(2)}\right\|_{L^2(\mathbb{R}^3)}\right) \le Ch, \tag{5.67}
$$

and there exists $\gamma' > 0$ such that for all $y \in \mathbb{R}^3$

$$
\begin{aligned}
&\sum_{|\alpha|\le 2}\left(|\partial^\alpha w_{h,k}(y)| + |\partial^\alpha \psi_{h,k}(y)|\right) \\
&\qquad \le C\left(\int_{\mathbb{R}^3}\left(\left|T_{h,k}^{(1)}(x)\right|^2 + \left|T_{h,k}^{(2)}(x)\right|^2\right)e^{-2\gamma'|x-y|}\,\mathrm{d}x\right)^{1/2}.
\end{aligned} \tag{5.68}
$$

The right-hand side of (5.68) can be estimated using (5.66) and the general form of Hölder's inequality

$$\begin{aligned}
&\int_{\mathbb{R}^3}\left(\left(T^{(1)}_{h,k}\right)^2(x)+\left(T^{(2)}_{h,k}\right)^2(x)\right)e^{-2\gamma'|x-y|}\,\mathrm{d}x\\
&\quad\le Ch\int_{\mathbb{R}^3}e^{-2\gamma'|x-y|}\prod_{i=1}^{k+1}|V_i|e^{-2\widetilde{\gamma}|x-Y_{n_i}|}\,\mathrm{d}x\\
&\quad= Ch\int_{\mathbb{R}^3}\prod_{i=1}^{k+1}|V_i|e^{-2\widetilde{\gamma}|x-Y_{n_i}|}e^{-2\gamma'/(k+1)|x-y|}\,\mathrm{d}x\\
&\quad\le Ch\prod_{i=1}^{k+1}|V_i|\left(\int_{\mathbb{R}^3}e^{-2(k+1)\widetilde{\gamma}|x-Y_{n_i}|}e^{-2\gamma'|x-y|}\,\mathrm{d}x\right)^{1/k+1}\\
&\quad\le Ch\prod_{i=1}^{k+1}|V_i|e^{-2\gamma|y-Y_{n_i}|},
\end{aligned}\tag{5.69}$$

where $\gamma=\gamma(\widetilde{\gamma},\gamma')>0$. Combining (5.68)–(5.69) gives

$$\sum_{|\alpha|\le 2}\left(|\partial^\alpha w_{h,k}(y)|+|\partial^\alpha\psi_{h,k}(y)|\right)\le Ch\prod_{i=1}^{k+1}|V_i|e^{-\gamma|y-Y_{n_i}|}.\tag{5.70}$$

We now pass to the limit in the system of equations (5.64) as $h\to 0$. As the functions $m_{\mathbf{V},\mathbf{n}}$, $R^{(1)}_{k,\mathbf{V},\mathbf{n}}$, $R^{(2)}_{k,\mathbf{V},\mathbf{n}}$ are all differentiable with respect to nuclear perturbations, it follows that

$$\frac{m_h-m_0}{h}\to m_{\mathbf{V}',\mathbf{n}'},\qquad \frac{T^{(1)}_{h,k}}{h}\to R^{(1)}_{k+1,\mathbf{V}',\mathbf{n}'},\qquad \frac{T^{(2)}_{h,k}}{h}\to R^{(2)}_{k+1,\mathbf{V}',\mathbf{n}'}\qquad \text{as } h\to 0,$$

and further (5.66) implies that $m_{\mathbf{V}',\mathbf{n}'}$, $R^{(1)}_{k+1,\mathbf{V}',\mathbf{n}'}$ and $R^{(2)}_{k+1,\mathbf{V}',\mathbf{n}'}$ satisfy (5.54)

$$\left|R^{(1)}_{k+1,\mathbf{V}',\mathbf{n}'}(x)\right|+\left|R^{(2)}_{k+1,\mathbf{V}',\mathbf{n}'}(x)\right|\le C\prod_{i=1}^{k}|V_i|e^{-\gamma|x-Y_{n_i}|}.$$

For any decreasing sequence $h_n\to 0$, then there exists a subsequence (still denoted by h_n) such that $\frac{w_{h_n,k}}{h_n}$ and $\frac{\psi_{h_n,k}}{h_n}$ converge to $\overline{w}\in H^4(\mathbb{R}^3)$ and $\overline{\psi}\in H^2(\mathbb{R}^3)$ respectively, weakly in $H^4(\mathbb{R}^3)$ and $H^2(\mathbb{R}^3)$, strongly in $H^3(B_R(0))$ and $H^1(B_R(0))$ for all $R>0$ and pointwise almost everywhere, along with their derivatives. In addition, it follows that $(\overline{w},\overline{\psi})$ solve the $k+1$-th variation of the TFW equations

$$
\begin{aligned}
-\Delta\overline{w} + \left(\frac{35}{9}u_0^{4/3} - \phi_0\right)\overline{w} - u_0\overline{\psi} &= R^{(1)}_{k+1,\mathbf{V}',\mathbf{n}'}, \\
-\Delta\overline{\psi} &= 4\pi\left(m_{\mathbf{V}',\mathbf{n}'} - 2u_0\overline{w}\right) + R^{(2)}_{k+1,\mathbf{V}',\mathbf{n}'}.
\end{aligned}
$$

As $u_0, \phi_0, m_{\mathbf{V}',\mathbf{n}'}, R^{(1)}_{k+1,\mathbf{V}',\mathbf{n}'}$ and $R^{(2)}_{k+1,\mathbf{V}',\mathbf{n}'}$ are independent of $(\overline{w},\overline{\psi})$, the uniqueness of this system of equations follows verbatim from the uniqueness of the linearised TFW equations [8, Corollary 2.3]. Consequently $(\overline{w},\overline{\psi})$ is independent of the choice of subsequence, hence $(\overline{w},\overline{\psi}) = (u_{\mathbf{V}'}, \phi_{\mathbf{V}',\mathbf{n}'})$. Moreover, passing to the limit in the estimates (5.67) and (5.70), it follows that $(u_{\mathbf{V}'}, \phi_{\mathbf{V}',\mathbf{n}'})$ satisfy (5.53) and (5.55)

$$
\sum_{|\alpha|\leq 2}\left(|\partial^\alpha\overline{u}(x)| + |\partial^\alpha\overline{\phi}(x)|\right) \leq C\prod_{i=1}^{k+1}|V_i|e^{-\gamma|x-Y_{n_i}|},
$$

and

$$
\begin{aligned}
&\|\overline{u}\|_{H^4(\mathbb{R}^3)} + \|\overline{\phi}\|_{H^2(\mathbb{R}^3)} \\
&\quad\leq C\left(\|m_{\mathbf{V}',\mathbf{n}'}\|_{L^2(\mathbb{R}^3)} + \left\|R^{(1)}_{k+1,\mathbf{V}',\mathbf{n}'}\right\|_{L^2(\mathbb{R}^3)} + \left\|R^{(2)}_{k+1,\mathbf{V}',\mathbf{n}'}\right\|_{L^2(\mathbb{R}^3)}\right).
\end{aligned}
$$

This completes the proof of the inductive step, hence the desired results hold for every variation of the TFW equations. □

Remark 18. It is straightforward to show an analogous result to Theorem 5.9 in the Yukawa setting, by following the proofs of Theorem 5.9 and Lemma 5.8. □

Proof of Corollary 5.10. We show Corollary 5.10 by adapting the proofs of Theorem 3.1, Corollary 3.9 and Lemma 5.6. As these results have been shown in detail already, due to the length of the argument involved, we only discuss the key steps of the proof.

Recall the space H^1_1, defined in (3.2), and let $\xi \in H^1_1$, that is $\xi \in H^1(\mathbb{R}^3)$ and $|\nabla\xi| \leq |\xi|$. Testing (5.64a) with $w\xi^2$, (5.64b) with $\frac{1}{8\pi}\psi\xi^2$ and adding these expressions and simplifying gives

$$\int_{\mathbb{R}^3}\left(|\nabla w|^2+\left(\frac{35}{9}u_0^{4/3}-\phi_0\right)w^2+|\nabla\psi|^2\right)\xi^2$$
$$\leq C\left(\int_{\mathbb{R}^3}(T_1w+T_2\psi)\,\xi^2+\int_{\mathbb{R}^3}(w^2+\psi^2)|\nabla\xi|^2\right). \tag{5.72}$$

The choice of test functions ensures that the coupling terms appearing in (5.64) cancel after summation, hence neither of them appear in the estimate (5.72).

Observe that

$$-\Delta w+\left(\frac{35}{9}u_0^{4/3}-\phi_0\right)w=Lw+\frac{20}{9}u_0^{4/3}w,$$

where $L=-\Delta+\frac{5}{3}u_0^{4/3}-\phi_0\geq 0$ by Lemma 2.9 and $\inf u_0\geq c_{M',\omega'}>0$ by Proposition 2.2. Using this, (5.72) can be simplified further

$$\int_{\mathbb{R}^3}\left(|\nabla w|^2+w^2+|\nabla\psi|^2\right)\xi^2$$
$$\leq C\left(\int_{\mathbb{R}^3}\left(T_1^2+T_2\psi\right)\xi^2+\int_{\mathbb{R}^3}(w^2+\psi^2)|\nabla\xi|^2\right). \tag{5.73}$$

We obtain an estimate for ψ^2 by testing (5.64a) with $\psi\xi^2$, which eventually yields

$$\int_{\mathbb{R}^3}\psi^2\xi^2\leq C\left(\int_{\mathbb{R}^3}\left(T_1^2+T_2^2\right)\xi^2+\int_{\mathbb{R}^3}(w^2+\psi^2)|\nabla\xi|^2\right). \tag{5.74}$$

Combining (5.73)–(5.74) implies

$$\int_{\mathbb{R}^3}\left(|\nabla w|^2+w^2+|\nabla\psi|^2+\psi^2\right)\xi^2$$
$$\leq C_0\left(\int_{\mathbb{R}^3}\left(T_1^2+T_2^2\right)\xi^2+\int_{\mathbb{R}^3}(w^2+\psi^2)|\nabla\xi|^2\right).$$

Consequently choosing $\gamma_0=\min\{1,(2C_0)^{-1/2}\}>0$ and $\xi\in H_{\gamma_0}$ allows us to remove the right hand term that depends on w,ψ to obtain

$$\int_{\mathbb{R}^3}\left(|\nabla w|^2+w^2+|\nabla\psi|^2+\psi^2\right)\xi^2\leq C\int_{\mathbb{R}^3}\left(T_1^2+T_2^2\right)\xi^2.$$

Following the proof of Lemma 3.7 gives an estimate of the form of (3.20), there exists $\gamma_0 > 0$ such that for all $y \in \mathbb{R}^3$

$$\sum_{|\alpha|\leq 2} |\partial^\alpha w(y)|^2 + \psi(y)^2 \leq C \int_{\mathbb{R}^3} \left(T_1^2(x) + T_2^2(x)\right) e^{-2\gamma_0|x-y|} \, \mathrm{d}x.$$

In fact, following the argument used to show (5.25) of Lemma 5.6 gives the desired result (5.57)

$$\sum_{|\alpha|\leq 2} \left(|\partial^\alpha w(y)|^2 + |\partial^\alpha \psi(y)|^2\right) \leq C \int_{\mathbb{R}^3} \left(T_1^2(x) + T_2^2(x)\right) e^{-2\gamma_0|x-y|} \, \mathrm{d}x.$$

Additionally, following the proof of Theorem 3.1 and (3.71) of Corollary 3.9 gives the remaining estimate (5.58)

$$\|w\|_{H^4(\mathbb{R}^3)} + \|\psi\|_{H^2(\mathbb{R}^3)} \leq C \left(\|T_1\|_{L^2(\mathbb{R}^3)} + \|T_2\|_{L^2(\mathbb{R}^3)}\right).$$

$\square$

Now that we have given a proof for Corollary 5.10, we are in a position to prove Lemma 5.7.

Proof of Lemma 5.7. The assumption (5.27) implies that $m_1 = m_2$ over $B_R(0)$, hence Proposition 4.1 yields: there exists $\gamma > 0$ such that for $|x| \leq R$

$$\sum_{|\alpha|\leq 2} |\partial^\alpha (u_1 - u_2)(x)| + |(\phi_1 - \phi_2)(y)| \leq C e^{-\gamma(R-|x|)}. \tag{5.75}$$

Also, the derivatives of m_1, m_2 with respect to their respective nuclear perturbations exist and satisfy

$$\begin{aligned} \overline{m}_1(x) = \frac{\partial m_1(Y_1; x)}{\partial Y_{1,j_1}} \cdot V = -\nabla \eta(x - Y_{1j_1}) \cdot V \\ = -\nabla \eta(x - Y_{2j_2}) \cdot V = \frac{\partial m_2(Y_2; x)}{\partial Y_{2,j_2}} \cdot V = \overline{m}_2(x), \end{aligned}$$

as $Y_{1j_1} = Y_{2j_2}$. Then, for $i = 1, 2$, applying Lemma 5.6, the variations defined in (5.28) exist and solve the linearised TFW equations

$$
\begin{aligned}
-\Delta \overline{u}_i + \left(\frac{35}{9} u_i^{4/3} - \phi_i\right) \overline{u}_i - u_i \overline{\phi}_i &= 0, \\
-\Delta \overline{\phi}_i &= 4\pi \left(\overline{m}_i - 2 u_i \overline{u}_i\right),
\end{aligned}
$$

and additionally there exists $\gamma_0 > 0$ such that

$$
\sum_{|\alpha| \leq 2} \left(|\partial^\alpha \overline{u}_i(x)| + |\partial^\alpha \overline{\phi}_i(x)|\right) \leq C|V| e^{-\gamma_0 |x - Y_{i j_i}|}, \tag{5.77}
$$

where the constant γ_0 is independent of $i = 1, 2$. Define $w = \overline{u}_1 - \overline{u}_2$ and $\psi = \overline{\phi}_1 - \overline{\phi}_2$, then combining the estimates (5.76) for $(\overline{u}_1, \overline{\phi}_1)$ and $(\overline{u}_2, \overline{\phi}_2)$ gives

$$
\begin{aligned}
-\Delta w + \left(\frac{35}{9} u_1^{4/3} - \phi_1\right) w - u_1 \psi &= T_1, \\
-\Delta \psi &= -8\pi u_1 w + T_2,
\end{aligned}
$$

where the residual terms are given by

$$
\begin{aligned}
T_1 &= \left(-\frac{35}{9}\left(u_1^{4/3} - u_2^{4/3}\right) + \phi_1 - \phi_2\right) \overline{u}_2 + (u_1 - u_2)\overline{\phi}_2, \\
T_2 &= -8\pi (u_1 - u_2) \overline{u}_2.
\end{aligned}
$$

Applying Proposition 2.1, (5.75) and (5.77), gives for $|x| \leq R$

$$
|T_1(x)| + |T_2(x)| \leq C|V| e^{-\gamma'(|x - Y_{1 j_1}| + R - |x|)}, \tag{5.79}
$$

and for $|x| > R$

$$
|T_1(x)| + |T_2(x)| \leq C|V| e^{-\gamma' |x - Y_{1 j_1}|}, \tag{5.80}
$$

where $\gamma' = \min\{\gamma, \gamma_0\} > 0$. Fix $|y| \leq R$ and by applying Corollary 5.10, there exists $\widetilde{\gamma} > 0$ such that

$$\sum_{|\alpha|\le 2} \left(|\partial^\alpha w(y)|^2 + |\partial^\alpha \psi(y)|^2\right) \le C \int_{\mathbb{R}^3} \left(|(T_1(x)|^2 + |T_2(x)|^2\right) e^{-2\widetilde{\gamma}|x-y|} \,\mathrm{d}x, \tag{5.81}$$

We decompose the right-hand side of (5.81) and apply (5.79)–(5.80) to obtain

$$\begin{aligned}
&\int_{\mathbb{R}^3} \left(|(T_1(x)|^2 + |T_2(x)|^2\right) e^{-2\widetilde{\gamma}|x-y|} \,\mathrm{d}x \\
&\le C|V| \int_{B_R(0)} e^{-2\gamma'(|x-Y_{1j_1}|+R-|x|)} e^{-2\widetilde{\gamma}|x-y|} \,\mathrm{d}x \\
&\qquad + C|V| \int_{B_R(0)^{\mathrm{c}}} e^{-2\gamma'|x-Y_{1j_1}|} e^{-2\widetilde{\gamma}|x-y|} \,\mathrm{d}x.
\end{aligned} \tag{5.82}$$

Let $\gamma_1 = \min\{\gamma', \frac{\widetilde{\gamma}}{3}\} > 0$, then the triangle inequality yields

$$\begin{aligned}
&e^{-2\gamma'(|x-Y_{1j_1}|+R-|x|)} e^{-2\widetilde{\gamma}|x-y|} \le e^{-2\gamma_1(|x-Y_{1j_1}|+R-|x|)} e^{-2\widetilde{\gamma}|x-y|} \\
&\le e^{-2\gamma_1(|y-Y_{1j_1}|+R-|y|)} e^{4\gamma_1|x-y|} e^{-2\widetilde{\gamma}|x-y|} \\
&\le e^{-2\gamma_1(|y-Y_{1j_1}|+R-|y|)} e^{-2\widetilde{\gamma}|x-y|/3},
\end{aligned}$$

which we use to estimate the first integral of (5.82)

$$\begin{aligned}
&\int_{B_R(0)} e^{-2\gamma'(|x-Y_{1j_1}|+R-|x|)} e^{-2\widetilde{\gamma}|x-y|} \,\mathrm{d}x \\
&\quad \le e^{-2\gamma_1(|y-Y_{1j_1}|+R-|y|)} \int_{B_R(0)} e^{-2\widetilde{\gamma}|x-y|/3} \,\mathrm{d}x \le Ce^{-2\gamma_1(|y-Y_{1j_1}|+R-|y|)}.
\end{aligned}$$

Let $d = R - |y|$, then the second integral can be estimated by

$$\begin{aligned}
&\int_{B_R(0)^{\mathrm{c}}} e^{-2\gamma'|x-Y_{1j_1}|} e^{-2\widetilde{\gamma}|x-y|} \,\mathrm{d}x \\
&\quad \le e^{-2\gamma_1|y-Y_{1j_1}|} \int_{B_R(0)^{\mathrm{c}}} e^{-4\widetilde{\gamma}|x-y|/3} \,\mathrm{d}x \le e^{-2\gamma_1|y-Y_{1j_1}|} \int_{B_d(y)^{\mathrm{c}}} e^{-4\widetilde{\gamma}|x-y|/3} \,\mathrm{d}x \\
&\quad \le Ce^{-2\gamma_1|y-Y_{1j_1}|}(1+d^2)e^{-4\widetilde{\gamma}d/3} \le Ce^{-2\gamma_1|y-Y_{1j_1}|} e^{-2\gamma_1 d}.
\end{aligned} \tag{5.83}$$

Collecting the estimates (5.81)–(5.83) gives the desired estimate (5.29)

$$\sum_{|\alpha|\le 2}\left(|\partial^\alpha w(y)|^2+|\partial^\alpha \psi(y)|^2\right)\le Ce^{-2\gamma_1(|y-Y_{1j_1}|+R-|y|)}.$$

□

5.6 Proofs and generalisation of Theorem 5.1

Using the notation of Definition 2 to define the derivatives of functions with respect to nuclear perturbations, we now state the general decay result for derivatives of the site energies.

Theorem 5.11. *Let $i=1,2$, $Y\in\mathcal{Y}_{L^2}(M,\omega)$ and $\{\varphi_j|j\in\mathbb{N}\}$ satisfy (5.6) and the following condition: there exists $k\in\mathbb{N},\widetilde{\gamma}>0$ such that for all $j\in\mathbb{N}$, $1\le k'\le k$, $\mathbf{n}=(n_1,\dots,n_{k'})\in\mathbb{N}^{k'}$, $\mathbf{V}\in(\mathbb{R}^3)^{k'}$ and $x\in\mathbb{R}^3$, the derivative*

$$\varphi_{j,\mathbf{V},\mathbf{n}}(Y;x)=\left\langle\frac{\partial^k\varphi_j(Y;x)}{\partial Y_{n_1}\cdots\partial Y_{n_{k'}}},\mathbf{V}\right\rangle$$

exists and satisfies

$$\left|\varphi_{j,\mathbf{V},\mathbf{n}}(Y;x)\right|\le Ce^{-\widetilde{\gamma}|x-Y_j|}\prod_{m=1}^{k'}|V_{n_m}|e^{-\widetilde{\gamma}|x-Y_{n_m}|}\tag{5.84}$$

Then it follows that $E_j^{(i)}$ is k-times differentiable with respect to nuclear perturbations and there exists $\gamma>0$ such that for all $\mathbf{n}=(n_1,\dots,n_{k'})\in\mathbb{N}^{k'}$ and $\mathbf{V}\in(\mathbb{R}^3)^{k'}$, $E^{(i)}_{j,\mathbf{V},\mathbf{n}}(Y)$ exists and satisfies

$$\left|E^{(i)}_{j,\mathbf{V},\mathbf{n}}(Y)\right|\le C\prod_{m=1}^{k}|V_{n_m}|e^{-\gamma|Y_j-Y_{n_m}|},\tag{5.85}$$

where $C=C(k',M,\omega,\widetilde{\gamma})$, $\gamma=\gamma(M,\omega,\widetilde{\gamma})>0$.

We now prove Theorem 5.1 and use this to prove Theorem 5.11.

Proof of Theorem 5.1. We will repeatedly use the fact that for all $\gamma_0,\widetilde{\gamma}>0$

there exist $C, \gamma > 0$ such that, for all $h \in [0, h_0]$, $p \in [1, 2]$,

$$\int_{\mathbb{R}^3} (1 + m_h(x) + |\nabla \phi_h(x)|)^p e^{-\gamma_0 |x - Y_n|} e^{-\widetilde{\gamma}|x - Y_j|} \, \mathrm{d}x \leq C e^{-\gamma |Y_j - Y_n|}. \tag{5.86}$$

In order to estimate the integral (5.86), let $\Gamma \subset \mathbb{R}^3$ be a semi-open unit cube centred at the origin. Then we may decompose $\mathbb{R}^3 = \{\Gamma + i | i \in \mathbb{Z}^3\}$. Then by (5.35), as $m_h, |\nabla \phi_h| \in L^2_{\mathrm{unif}}(\mathbb{R}^3)$, there exists $\gamma > 0$ such that

$$\begin{aligned}
&\int_{\mathbb{R}^3} (1 + m_h(x) + |\nabla \phi_h(x)|)^p e^{-\gamma_0 |x - Y_n|} e^{-\widetilde{\gamma}|x - Y_j|} \, \mathrm{d}x \\
&\qquad = C \sum_{i \in \mathbb{Z}^3} \int_{\Gamma + i} (1 + m_h(x) + |\nabla \phi_h(x)|)^p e^{-\gamma_0 |x - Y_n|} e^{-\widetilde{\gamma}|x - Y_j|} \, \mathrm{d}x \\
&\qquad \leq C \sum_{i \in \mathbb{Z}^3} \|1 + m_h + |\nabla \phi_h|\|^p_{L^2(\Gamma + i)} \|e^{-\gamma_0 |\cdot - Y_n|} e^{-\widetilde{\gamma}|\cdot - Y_j|}\|_{L^{\frac{2}{2-p}}(\Gamma + i)} \\
&\qquad \leq C |\Gamma|^{1/2} \sum_{i \in \mathbb{Z}^3} \|1 + m_h + |\nabla \phi_h|\|^2_{L^2(\Gamma + i)} e^{-\gamma_0 |i - Y_n|} e^{-\widetilde{\gamma}|i - Y_j|} \\
&\qquad \leq C(1 + M_1)^2 \sum_{i \in \mathbb{Z}^3} e^{-\gamma_0 |i - Y_n|} e^{-\widetilde{\gamma}|i - Y_j|} \leq C e^{-\gamma |Y_j - Y_n|}.
\end{aligned}$$

Further, we also use that for all $j \in \mathbb{N}$, $h \in (0, h_0]$, $x \in \mathbb{R}^3$,

$$\left| \frac{\varphi_j(Y^h; x) - \varphi_j(Y; x)}{h} \right| \leq C e^{-\widetilde{\gamma}|x - Y_j|} e^{-\widetilde{\gamma}|x - Y_n|}, \tag{5.87}$$

which follows from (5.6c). By (5.16), for all $j \in \mathbb{N}$ $Y^h_j - Y_j = \delta_{jn} h V$, and since $\varphi_j(Y; x)$ is differentiable with respect to Y_n, by the Mean Value Theorem, there exists $h^* \in (0, h) \subset [0, h_0]$ such that

$$\frac{\varphi(Y^h; x) - \varphi(Y; x)}{h} = \frac{\partial \varphi(Y^{h^*}; x)}{\partial Y_n} \cdot V.$$

Consequently, Lemma 5.3 implies $Y^{h^*} \in \mathcal{Y}_{L^2}(M_1, \omega_1)$, hence by (5.6c) there exists $C, \widetilde{\gamma} > 0$ such that

$$\left| \frac{\varphi(Y^h; x) - \varphi(Y; x)}{h} \right| \leq |V| \left| \frac{\partial \varphi(Y^{h^*}; x)}{\partial Y_n} \right| \leq C |V| e^{-\widetilde{\gamma}|x - Y^{h^*}_j|} e^{-\widetilde{\gamma}|x - Y^{h^*}_n|}.$$

Since for each $j' \in \mathbb{N}$ $|Y^{h^*}_{j'} - Y_{j'}| \leq h_0 |V| \leq 1$, we obtain (5.87) by applying the triangle inequality

$$\left|\frac{\varphi(Y^h;x)-\varphi(Y;x)}{h}(Y;x)\right| \leq C|V|e^{-\widetilde{\gamma}|x-Y_j^{h^*}|}e^{-\widetilde{\gamma}|x-Y_n^{h^*}|}$$
$$\leq Ce^{2\widetilde{\gamma}}|V|e^{-\widetilde{\gamma}|x-Y_j|}e^{-\widetilde{\gamma}|x-Y_n|}.$$

For $i=1,2$ and $j\in\mathbb{N}$, consider the difference

$$\frac{E_j^{(i)}(Y^h)-E_j^{(i)}(Y)}{h} = \int_{\mathbb{R}^3} \frac{\mathcal{E}_i(Y^h;x)\varphi_j(Y^h;x)-\mathcal{E}_i(Y;x)\varphi_j(Y;x)}{h}\,\mathrm{d}x$$
$$= \int_{\mathbb{R}^3}\left(\frac{\mathcal{E}_i(Y^h;x)-\mathcal{E}_i(Y;x)}{h}\right)\varphi_j(Y^h;x)\,\mathrm{d}x$$
$$+ \int_{\mathbb{R}^3}\mathcal{E}_i(Y;x)\left(\frac{\varphi_j(Y^h;x)-\varphi_j(Y;x)}{h}\right)\,\mathrm{d}x \tag{5.88}$$

We wish to show that the limit of (5.88) exists as $h\to 0$ to obtain

$$\frac{\partial E_j^{(i)}}{\partial Y_n} = \int_{\mathbb{R}^3}\frac{\partial\mathcal{E}_i}{\partial Y_n}(Y;x)\varphi_j(Y;x)\,\mathrm{d}x + \int_{\mathbb{R}^3}\mathcal{E}_i(Y;x)\frac{\partial\varphi_j}{\partial Y_n}(Y;x)\,\mathrm{d}x, \tag{5.89}$$

where

$$\frac{\partial\mathcal{E}_1}{\partial Y_n}(Y;\cdot) = 2\nabla u\cdot\nabla\overline{u} + \frac{10}{3}u^{7/3}\overline{u} + \frac{1}{2}\overline{\phi}(m-u^2) + \frac{1}{2}\phi(\overline{m}-2u\overline{u}), \tag{5.90}$$
$$\frac{\partial\mathcal{E}_2}{\partial Y_n}(Y;\cdot) = 2\nabla u\cdot\nabla\overline{u} + \frac{10}{3}u^{7/3}\overline{u} + \frac{1}{4\pi}\nabla\overline{\phi}\cdot\nabla\phi. \tag{5.91}$$

Case 1. First consider the energy density

$$\mathcal{E}_1(Y;x) = |\nabla u(x)|^2 + u^{10/3}(x) + \frac{1}{2}\phi(x)(m-u^2)(x). \tag{5.92}$$

To show (5.90), consider the difference

$$\begin{aligned}\frac{\mathcal{E}_1(Y^h;\cdot)-\mathcal{E}_1(Y;\cdot)}{h} &= \nabla(u_h+u)\cdot\nabla\left(\frac{u_h-u}{h}\right)+\left(\frac{u_h^{10/3}-u^{10/3}}{h}\right)\\ &\quad+\frac{1}{2h}\left(\phi_h(m_h-u_h^2)-\frac{1}{2}\phi(m-u^2)\right)\\ &= \nabla(u_h+u)\cdot\nabla\left(\frac{u_h-u}{h}\right)+\left(\frac{u_h^{10/3}-u^{10/3}}{h}\right)\\ &\quad+\frac{1}{2}\left(\frac{\phi_h-\phi}{h}\right)(m-u^2)+\frac{1}{2}\phi_h\left(\frac{m_h-m-u_h^2+u^2}{h}\right).\end{aligned} \tag{5.93}$$

It follows from (5.93) and pointwise convergence of $u_h, \nabla u_h, \phi_h$ to $u, \nabla u, \phi$ and $\frac{u_h-u}{h}, \nabla\left(\frac{u_h-u}{h}\right), \frac{\phi_h-\phi}{h}, \frac{m_h-m}{h}$ to $\overline{u}, \nabla\overline{u}, \overline{\phi}, \overline{m}$ as $h \to 0$, that (5.90) holds

$$\begin{aligned}&\lim_{h\to 0}\frac{\mathcal{E}_1(Y^h;\cdot)-\mathcal{E}_1(Y;\cdot)}{h}\\ &\quad= 2\nabla u\cdot\nabla\overline{u}+\frac{10}{3}u^{7/3}\overline{u}+\frac{1}{2}\overline{\phi}(m-u^2)+\frac{1}{2}\phi(\overline{m}-2u\overline{u})=\frac{\partial\mathcal{E}_1}{\partial Y_n}.\end{aligned}$$

Applying (5.22) to (5.93) yields

$$\begin{aligned}&\left|\mathcal{E}_1(Y^h;x)-\mathcal{E}_1(Y;x)\right|\\ &\quad\le C\left(|(u_h-u)(x)|+|\nabla(u_h-u)(x)|+|(m_h-m)(x)|\right)\\ &\qquad\quad+C(1+m(x))|(\phi_h-\phi)(x)|\\ &\quad\le Ch(1+m(x))e^{-\gamma_0|x-Y_n|}.\end{aligned} \tag{5.94}$$

Combining (5.94) and (5.6b), we deduce

$$\left|\frac{\mathcal{E}_1(Y^h;x)-\mathcal{E}_1(Y;x)}{h}\varphi_j(Y;x)\right| \le C(1+m(x))e^{-\gamma_0|x-Y_n|}e^{-\widetilde{\gamma}|x-Y_j|}, \tag{5.95}$$

hence by (5.86) and the Dominated Convergence Theorem,

$$\int_{\mathbb{R}^3}\frac{\partial\mathcal{E}_1}{\partial Y_n}(Y;x)\varphi_j(Y;x)\,\mathrm{d}x=\lim_{h\to 0}\int_{\mathbb{R}^3}\left(\frac{\mathcal{E}_1(Y^h;x)-\mathcal{E}_1(Y;x)}{h}\right)\varphi_j(Y;x)\,\mathrm{d}x. \tag{5.96}$$

It follows from (5.95) and (5.86) that

$$\left|\int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_1}{\partial Y_n}(Y;x)\varphi_j(Y;x)\, \mathrm{d}x\right| \le C\int_{\mathbb{R}^3}(1+m(x))e^{-\gamma_0|x-Y_n|}e^{-\widetilde{\gamma}|x-Y_j|}\,\mathrm{d}x$$
$$\le Ce^{-\gamma|Y_j-Y_n|}. \tag{5.97}$$

It remains to show that (5.88) converges using (5.86) and (5.87). As $\varphi_j(Y;x)$ is differentiable with respect to Y_n, for all $x\in\mathbb{R}^3$

$$\mathcal{E}_1(Y;x)\,\frac{\partial\varphi_j}{\partial Y_n}(Y;x) = \lim_{h\to 0}\mathcal{E}_1(Y;x)\left(\frac{\varphi_j(Y^h;x)-\varphi_j(Y;x)}{h}\right),$$

and combining (5.92) with (5.87) implies

$$\left|\mathcal{E}_1(Y;x)\left(\frac{\varphi_j(Y^h;x)-\varphi_j(Y;x)}{h}\right)\right| \le C(1+m(x))e^{-\gamma_0|x-Y_n|}e^{-\widetilde{\gamma}|x-Y_j|},$$

hence by (5.86) and the Dominated Convergence Theorem,

$$\int_{\mathbb{R}^3}\mathcal{E}_1(Y;x)\frac{\partial\varphi_j}{\partial Y_n}(Y;x)\,\mathrm{d}x = \lim_{h\to0}\int_{\mathbb{R}^3}\mathcal{E}_1(Y;x)\left(\frac{\varphi_j(Y^h;x)-\varphi_j(Y;x)}{h}\right)\,\mathrm{d}x,$$
$$\text{and}\qquad \left|\int_{\mathbb{R}^3}\mathcal{E}_1(Y;x)\frac{\partial\varphi_j}{\partial Y_n}(Y;x)\,\mathrm{d}x\right| \le Ce^{-\gamma|Y_j-Y_n|}. \tag{5.98}$$

Combining (5.97) and (5.98) yields the desired estimate (5.8).
Case 2. Now consider the energy density

$$\mathcal{E}_2(x) = |\nabla u(x)|^2 + u^{10/3}(x) + \frac{1}{8\pi}|\nabla\phi(x)|^2.$$

To show (5.89), as we have shown (5.96)–(5.97) in Case 1, we now prove

$$\lim_{h\to0}\frac{1}{8\pi h}\int_{\mathbb{R}^3}\left(|\nabla\phi_h|^2-|\nabla\phi|^2\right)(x)\varphi_j(Y^h;x)$$
$$= \frac{1}{4\pi}\int_{\mathbb{R}^3}\nabla\overline{\phi}(x)\cdot\nabla\phi(x)\varphi_j(Y;x)\,\mathrm{d}x, \tag{5.99}$$
$$\left|\frac{1}{4\pi}\int_{\mathbb{R}^3}\nabla\overline{\phi}(x)\cdot\nabla\phi(x)\varphi_j(Y;x)\,\mathrm{d}x\right| \le Ce^{-\gamma|Y_j-Y_n|}. \tag{5.100}$$

As

$$\frac{1}{8\pi h}\int_{\mathbb{R}^3}\left(|\nabla\phi_h|^2-|\nabla\phi|^2\right)(x)\varphi_j(Y^h;x)\,\mathrm{d}x$$
$$=\frac{1}{8\pi}\int_{\mathbb{R}^3}\nabla\left(\frac{\phi_h-\phi}{h}\right)(x)\cdot\nabla(\phi_h+\phi)(x)\varphi_j(Y^h;x)\,\mathrm{d}x,$$

it follows from (5.22) and (5.86) that

$$\left|\frac{1}{8\pi h}\int_{\mathbb{R}^3}\left(|\nabla\phi_h|^2-|\nabla\phi|^2\right)(x)\varphi_j(Y^h;x)\,\mathrm{d}x\right|$$
$$\leq C\int_{\mathbb{R}^3}(|\nabla\phi(x)|+|\nabla\phi(x)|)e^{-\gamma_0|x-Y_n|}e^{-\widetilde{\gamma}|x-Y_j|}\,\mathrm{d}x\leq Ce^{-\gamma|Y_j-Y_n|},$$

so (5.99)–(5.100) follow by the Dominated Convergence Theorem. Combining the estimates (5.99) with (5.96) yields (5.91) and

$$\int_{\mathbb{R}^3}\frac{\partial\mathcal{E}_2}{\partial Y_n}(Y;x)\varphi_j(Y;x)\,\mathrm{d}x=\lim_{h\to0}\int_{\mathbb{R}^3}\left(\frac{\mathcal{E}_2(Y^h;x)-\mathcal{E}_2(Y;x)}{h}\right)\varphi_j(Y^h;x)\,\mathrm{d}x.$$

and (5.100) with (5.97) yields

$$\left|\int_{\mathbb{R}^3}\frac{\partial\mathcal{E}_2}{\partial Y_n}(Y;x)\varphi_j(Y;x)\right|\leq C\int_{\mathbb{R}^3}(1+|\nabla\phi(x)|)e^{-\gamma_0|x-Y_n|}e^{-\widetilde{\gamma}|x-Y_j|}\,\mathrm{d}x$$
$$\leq Ce^{-\gamma|Y_j-Y_n|}.$$

It remains to show that (5.88) converges using (5.86) and (5.87). As $\varphi_j(Y;x)$ is differentiable with respect to Y_n, for all $x\in\mathbb{R}^3$

$$\mathcal{E}_2(Y;x)\frac{\partial\varphi_j}{\partial Y_n}(Y;x)=\lim_{h\to0}\mathcal{E}_2(Y;x)\left(\frac{\varphi_j(Y^h;x)-\varphi_j(Y;x)}{h}\right),$$

and applying (5.86) yields

$$\left|\int_{\mathbb{R}^3}\mathcal{E}_2(Y;x)\left(\frac{\varphi_j(Y^h;x)-\varphi_j(Y;x)}{h}\right)\right|$$
$$\leq C\int_{\mathbb{R}^3}(1+|\nabla\phi(x)|^2)e^{-\gamma_0|x-Y_n|}e^{-\widetilde{\gamma}|x-Y_j|}\,\mathrm{d}x\leq Ce^{-\gamma|Y_j-Y_n|},$$

hence by the Dominated Convergence Theorem

$$\int_{\mathbb{R}^3} \mathcal{E}_2(Y;x)\,\frac{\partial \varphi_j}{\partial Y_n}(Y;x)\;\mathrm{d}x = \lim_{h\to 0}\int_{\mathbb{R}^3} \mathcal{E}_2(Y;x)\left(\frac{\varphi_j(Y^h;x)-\varphi_j(Y;x)}{h}\right)\;\mathrm{d}x$$

and

$$\left|\int_{\mathbb{R}^3} \mathcal{E}_2(Y;x)\,\frac{\partial \varphi_j}{\partial Y_n}(Y;x)\;\mathrm{d}x\right| \le Ce^{-\gamma|Y_j-Y_n|}. \tag{5.101}$$

Combining (5.98) and (5.101), the desired estimate (5.8) holds

$$\left|\frac{\partial E_j^{(2)}}{\partial Y_n}\right| \le Ce^{-\gamma|Y_j-Y_n|}.$$

□

We now show (5.9), that the two energy densities generate an indentical force.

Proof of (5.9). To prove (5.9), we require that

$$\sum_{j\in\mathbb{N}} e^{-\gamma|Y_j-Y_m|} < \infty, \tag{5.102}$$

which holds as $Y \in \mathcal{Y}_{L^2}(M,\omega)$. To show this, for $n \in \mathbb{N}$ define

$$A_n(Y_m) := \{j \in \mathbb{N} | n-1 < |Y_j - Y_m| < n\},$$

which satisfies

$$|A_n(Y_m)| \le \int_{B_{n+R_0}(Y_m)} m_Y(z)\;\mathrm{d}z \le |B_{n+R_0}(Y_m)|\|m_Y\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \le CM_1(1+n^3),$$

where $C = C(R_0) > 0$. Then (5.102) holds as

$$\sum_{j\in\mathbb{N}} e^{-\gamma|Y_j-Y_m|} = \sum_{n\in\mathbb{N}}\sum_{j\in A_n(Y_m)} e^{-\gamma|Y_j-Y_m|} \le C\sum_{n\in\mathbb{N}}(1+n^3)e^{-\gamma n} < \infty.$$

Then for $i \in \{1,2\}$

$$\sum_{j\in\mathbb{N}} \left| \frac{\partial E_j^{(i)}}{\partial Y_n} \right| \le \sum_{j\in\mathbb{N}} \left| \int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_i}{\partial Y_n}(Y;x)\varphi_j(Y;x)\,\mathrm{d}x \right| + \sum_{j\in\mathbb{N}} \left| \int_{\mathbb{R}^3} \mathcal{E}_i(Y;x)\frac{\partial \varphi_j}{\partial Y_n}(Y;x)\,\mathrm{d}x \right| \le C\sum_{j\in\mathbb{N}} e^{-\gamma|Y_j-Y_n|} < \infty,$$

hence by the Monotone Convergence Theorem, the sum is well-defined

$$\sum_{j\in\mathbb{N}} \frac{\partial E_j^{(1)}}{\partial Y_n} = \int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_i}{\partial Y_n}(Y;x)\left(\sum_{j\in\mathbb{N}} \varphi_j(Y;x)\right)\,\mathrm{d}x + \int_{\mathbb{R}^3} \mathcal{E}_i(Y;x)\left(\sum_{j\in\mathbb{N}} \frac{\partial \varphi_j}{\partial Y_n}(Y;x)\right)\,\mathrm{d}x.$$

As $(\varphi_j)_{j\in\mathbb{N}}$ satisfies (5.6a) for all $h \in [0,h_0]$, it follows that

$$\sum_{j\in\mathbb{N}} \frac{\partial \varphi_j}{\partial Y_n}(Y;x) = 0,$$

and consequently,

$$\sum_{j\in\mathbb{N}} \frac{\partial E_j^{(i)}}{\partial Y_n} = \int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_i}{\partial Y_n}(Y;x)\,\mathrm{d}x.$$

Now consider the difference of (5.90)–(5.91)

$$\left(\frac{\partial \mathcal{E}_1}{\partial Y_n} - \frac{\partial \mathcal{E}_2}{\partial Y_n}\right)(Y;\cdot) = \frac{1}{2}\overline{\phi}(m-u^2) + \frac{1}{2}\phi(\overline{m}-2u\overline{u}) - \frac{1}{4\pi}\nabla\overline{\phi}\cdot\nabla\phi,$$

and applying integration by parts yields

$$
\begin{aligned}
\int_{\mathbb{R}^3} \left(\frac{\partial \mathcal{E}_1}{\partial Y_n} - \frac{\partial \mathcal{E}_2}{\partial Y_n} \right) (Y; x) \, \mathrm{d}x \\
&= \int_{\mathbb{R}^3} \left(\frac{1}{2} \overline{\phi}(m - u^2) + \frac{1}{2} \phi(\overline{m} - 2u\overline{u}) - \frac{1}{4\pi} \nabla \overline{\phi} \cdot \nabla \phi \right) \\
&= \frac{1}{8\pi} \int_{\mathbb{R}^3} \left(\overline{\phi}(-\Delta \phi) + \phi(-\Delta \overline{\phi}) - 2 \nabla \overline{\phi} \cdot \nabla \phi \right) \\
&= \frac{1}{8\pi} \int_{\mathbb{R}^3} \left(2 \nabla \overline{\phi} \cdot \nabla \phi - 2 \nabla \overline{\phi} \cdot \nabla \phi \right) = 0.
\end{aligned}
$$

In addition, since

$$
\frac{1}{4\pi} \int_{\mathbb{R}^3} \nabla \phi \cdot \nabla \overline{\phi} = \frac{1}{4\pi} \int_{\mathbb{R}^3} \phi(-\Delta \overline{\phi}) = \int_{\mathbb{R}^3} \phi(\overline{m} - 2u\overline{u})
$$

and since u solves (2.2a), $-\Delta u + \frac{5}{3} u^{7/3} - \phi u = 0$, the desired result (5.9) holds:

$$
\int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_2}{\partial Y_n}(Y; x) \, \mathrm{d}x = 2 \int_R \left(\nabla u \cdot \nabla \overline{u} + \frac{5}{3} u^{7/3} \overline{u} - \phi u \overline{u} \right) + \int_{\mathbb{R}^3} \phi \, \overline{m} = \int_{\mathbb{R}^3} \phi \, \overline{m}.
$$

□

Proof of Theorem 5.11. We argue by induction and follow the argument used to prove Theorem 5.1. Let $i \in \{1, 2\}$. Recall the assumption that for all $j \in \mathbb{N}$, φ_j is k-times differentiable with respect to nuclear perturbations and also satisfies the decay estimate (5.84). In addition, as $\mathcal{E}_i$ are functions of $u, \nabla u, \phi, \nabla \phi, m$, it follows as a direct consequence of Theorem 5.9 and (5.50)–(5.51) that $\mathcal{E}_i$ is infinitely-differentiable with respect to nuclear perturbations. Moreover, for all $s \in \mathbb{N}$ there exists $C = C_s, \gamma > 0$ such that for all $\mathbf{V} \in (\mathbb{R}^3)^s$ and $\mathbf{n} \in \mathbb{N}^s$

$$
\left| \mathcal{E}_{i,\mathbf{V},\mathbf{n}}(Y; x) \right| \leq C \prod_{i=1}^{s} |V_m| e^{-\gamma |x - Y_{n_m}|}. \tag{5.103}
$$

Fix $j \in \mathbb{N}$ and suppose that for some $1 \leq k' \leq k-1$, $E_j^{(i)}$ is k'-times differentiable and that for all $Y \in \mathcal{Y}_{L^2}(M, \omega)$, $\mathbf{V} \in (\mathbb{R}^3)^{k'}$ and $\mathbf{n} \in \mathbb{N}^{k'}$

$$
E^{(i)}_{j,\mathbf{V},\mathbf{n}}(Y) = \int_{\mathbb{R}^3} \left(\mathcal{E}_i \, \varphi_j \right)_{\mathbf{V},\mathbf{n}} (Y; x) \, \mathrm{d}x.
$$

Observe that the case $k' = 1$ has been shown in Theorem 5.1. Now let $V_{k'+1} \in \mathbb{R}^3$, $n_{k'+1} \in \mathbb{N}$ and define $\mathbf{V}' \in (\mathbb{R}^3)^{k'+1}, \mathbf{n}' \in \mathbb{N}^{k'+1}$ such that $\mathbf{V}' = (\mathbf{V}, V_{k'+1}), \mathbf{n}' = (\mathbf{n}, n_{k'+1})$. In addition, let $Y \in \mathcal{Y}_{L^2}(M,\omega)$, then let $h_0 = (1 + |V_{k'+1}|)^{-1}$ and for $h \in [0, h_0]$, define

$$Y^h = \{\, Y_j + \delta_{n_{k'+1}}(j) h V_{k'+1} \,|\, j \in \mathbb{N} \,\}.$$

Applying the Mean Value Theorem, there exists $h^* \in (0, h)$ satisfying

$$\begin{aligned} \frac{E^{(i)}_{j,\mathbf{V},\mathbf{n}}(Y^h) - E^{(i)}_{j,\mathbf{V},\mathbf{n}}(Y)}{h} &= \int_{\mathbb{R}^3} \frac{(\mathcal{E}_i\,\varphi_j)_{\mathbf{V},\mathbf{n}}(Y^h; x) - (\mathcal{E}_i\,\varphi_j)_{\mathbf{V},\mathbf{n}}(Y; x)}{h}\, \mathrm{d}x \\ &= \int_{\mathbb{R}^3} (\mathcal{E}_i\,\varphi_j)_{\mathbf{V}',\mathbf{n}'}(Y^{h^*}; x)\, \mathrm{d}x. \end{aligned} \tag{5.104}$$

Now applying (5.84), (5.103) and Lemma 5.3, we deduce that

$$\left| (\mathcal{E}_i\,\varphi_j)_{\mathbf{V}',\mathbf{n}'}(Y^{h^*}; x) \right| \leq C e^{-\widetilde{\gamma}|x - Y_j|} \prod_{m=1}^{k'+1} |V_m| e^{-\gamma_0 |x - Y_{n_m}|},$$

independently of h, hence by the Dominated Convergence Theorem, sending $h \to 0$ in (5.104) yields

$$E^{(i)}_{j,\mathbf{V}',\mathbf{n}'}(Y) = \int_{\mathbb{R}^3} (\mathcal{E}_i\,\varphi_j)_{\mathbf{V}',\mathbf{n}'}(Y; x)\, \mathrm{d}x,$$

and moreover

$$\left| E^{(i)}_{j,\mathbf{V}',\mathbf{n}'}(Y) \right| \leq C \int_{\mathbb{R}^3} e^{-\widetilde{\gamma}|x - Y_j|} \prod_{m=1}^{k'+1} |V_m| e^{-\gamma_0|x - Y_{n_m}|}\, \mathrm{d}x \leq C \prod_{m=1}^{k'+1} |V_m| e^{-\gamma |Y_j - Y_{n_m}|}. \tag{5.105}$$

This completes the proof of the inductive step, hence the desired result (5.85) follows from (5.105) by choosing $k' = k - 1$. ∎

We now use Lemma 5.8 and Theorem 5.1 to prove Theorem 5.2.

Proof of Theorem 5.2. Let $0 < a \leq a_0$ and $h \in [0, h_0]$, then recall (5.13)

$$\mathcal{E}_{2,a}(Y^h; \cdot) = |\nabla u_{a,h}|^2 + u_{a,h}^{10/3} + \tfrac{1}{8\pi}\left(|\nabla \phi_{a,h}|^2 + a^2 \phi_{a,h}^2 \right).$$

Applying Lemma 5.8 and using the pointwise convergence of $u_{a,h}, \phi_{a,h}$, $\frac{u_{a,h}-u_a}{h}, \frac{\phi_{a,h}-\phi_a}{h}$ to $u_a, \phi_a, \overline{u}_a, \overline{\phi}_a$ as $h \to 0$, along with their derivatives, it follows that

$$\frac{\mathcal{E}_{2,a}(Y^h;\cdot) - \mathcal{E}_{2,a}(Y;\cdot)}{h} \to 2\nabla u_a \cdot \nabla \overline{u}_a + \frac{10}{3} u_a^{7/3}\, \overline{u}_a + \frac{1}{4\pi}\left(\nabla \phi_a \cdot \nabla \overline{\phi}_a + a^2 \phi_a \overline{\phi}_a\right).$$

As $u_a \in W^{1,\infty}(\mathbb{R}^3)$, $\phi_a \in L^\infty(\mathbb{R}^3)$, $\nabla \phi_a \in L^2_{\text{unif}}(\mathbb{R}^3)$ and (5.33) holds

$$\sum_{|\alpha| \le 2} \left(|\partial^\alpha \overline{u}_a(x)| + |\partial^\alpha \overline{\phi}_a(x)|\right) + |\overline{m}(x)| \le C e^{-\gamma_0 |x - Y_k|},$$

it follows that $\partial_{Y_k} \mathcal{E}_{2,a} \in L^1(\mathbb{R}^3)$ and

$$\begin{aligned}\int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_{2,a}(Y;x)}{\partial Y_k}\, \mathrm{d}x = 2\int_{\mathbb{R}^3} \nabla u_a \cdot \nabla \overline{u}_a + \frac{10}{3}\int_{\mathbb{R}^3} u_a^{7/3} \overline{u}_a \\ + \frac{1}{4\pi}\int_{\mathbb{R}^3} \left(\nabla \phi_a \cdot \nabla \overline{\phi}_a + a^2 \phi_a \overline{\phi}_a\right).\end{aligned} \tag{5.106}$$

An identical argument shows that $\partial_{Y_k} \mathcal{E}_{1,a} \in L^1(\mathbb{R}^3)$ and

$$\begin{aligned}\int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_{1,a}(Y;x)}{\partial Y_k}\, \mathrm{d}x = 2\int_{\mathbb{R}^3} \nabla u_a \cdot \nabla \overline{u}_a + \frac{10}{3}\int_{\mathbb{R}^3} u_a^{7/3} \overline{u}_a \\ + \frac{1}{2}\int_{\mathbb{R}^3} \left(\phi_a(\overline{m} - 2u_a \overline{u}_a) + \overline{\phi}_a(m - u_a^2)\right).\end{aligned}$$

Using that ϕ_a and $\overline{\phi}_a$ solve (2.3b) and (5.32b), respectively,

$$\begin{aligned}\frac{1}{2}\int_{\mathbb{R}^3} \overline{\phi}_a(m - u_a^2) &= \frac{1}{8\pi}\int_{\mathbb{R}^3} \overline{\phi}_a(-\Delta \phi_a + a^2 \phi_a) = \frac{1}{8\pi}\int_{\mathbb{R}^3} \left(\nabla \phi_a \cdot \nabla \overline{\phi}_a + a^2 \phi_a \overline{\phi}_a\right) \\ &= \frac{1}{8\pi}\int_{\mathbb{R}^3} \phi_a(-\Delta \overline{\phi}_a + a^2 \overline{\phi}_a) = \frac{1}{2}\int_{\mathbb{R}^3} \phi_a(\overline{m} - 2u_a \overline{u}_a).\end{aligned} \tag{5.107}$$

Combining (5.106)–(5.107) and using that u_a solves $-\Delta u_a + \frac{5}{3} u_a^{7/3} - \phi_a u_a = 0$

(2.3a), the estimate (5.14) follows

$$\int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_{1,a}(Y;x)}{\partial Y_k}\,\mathrm{d}x = \int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_{2,a}(Y;x)}{\partial Y_k}\,\mathrm{d}x$$
$$= 2\left(\int_{\mathbb{R}^3} \nabla u_a \cdot \nabla \overline{u}_a + \frac{5}{3}\int_{\mathbb{R}^3} u_a^{7/3}\overline{u}_a - \int_{\mathbb{R}^3} \phi_a u_a \overline{u}_a\right) + \int_{\mathbb{R}^3} \phi_a \overline{m} = \int_{\mathbb{R}^3} \phi_a \overline{m}.$$

Now recall the corresponding result for the Coulomb case (5.9), that $\partial_{Y_k}\mathcal{E}_1$, $\partial_{Y_k}\mathcal{E}_2 \in L^1(\mathbb{R}^3)$ and

$$\int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_1(Y;x)}{\partial Y_k}\,\mathrm{d}x = \int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_2(Y;x)}{\partial Y_k}\,\mathrm{d}x = \int_{\mathbb{R}^3} \phi\,\overline{m}.$$

Applying (4.13) of Theorem 4.4 and (5.33) of Lemma 5.8 yields the desired estimate (5.15), for $i \in \{1, 2\}$

$$\left|\int_{\mathbb{R}^3} \left(\frac{\partial \mathcal{E}_{i,a}}{\partial Y_k} - \frac{\partial \mathcal{E}_i}{\partial Y_k}\right)(Y;x)\,\mathrm{d}x\right|$$
$$\leq \int_{\mathbb{R}^3} |\phi_a - \phi||\overline{m}| \leq C\|\phi_a - \phi\|_{L^\infty(\mathbb{R}^3)} \int_{\mathbb{R}^3} e^{-\gamma|x-Y_k|}\,\mathrm{d}x \leq Ca^2. \square$$

Chapter 6

The Lattice Relaxation Problem

The aim of this chapter is to use the site energies introduced in Section 1.1 and defined in (1.6) to study the relaxation of a perfect lattice in the presence of point defects using the TFW energy. This problem was introduced in [23] in the context of site potentials with finite interaction range, treating both point defects and dislocations. We refer the reader to Section 1.1, which discusses the challenges and techniques required to extend the analysis presented in [23, Sections 5, 6] to the TFW model.

We adapt the analysis presented in [23] to the TFW model by applying the model for point defects formulated in [23, Section 2.1] to obtain a decay result similar to [23, Theorem 2.3]. The locality estimates established in Chapter 5 are crucial in our analysis as they allow us to control the infinite-range interaction of the TFW model within the variational framework introduced in [23].

The analysis presented in this chapter can be applied to other models satisfying the exponential locality property, such as the tight binding model with Yukawa interaction [17]. Moreover, in forthcoming work [2], we establish the minimal decay conditions for a site energy that ensures the lattice relaxation problem can be defined, considering the lattice relaxation caused by either point defects or dislocations.

We now outline the construction of the lattice relaxation problem and state the main results. The proofs of these results can be found in Sections 6.6–6.10.

6.1 Modelling point defects

We consider a point defect embedded in a homogeneous crystalline bulk. Let $A \in \mathbb{R}^{3\times 3}$ be nonsingular, then a homogeneous crystal reference configuration is given by the Bravais lattice $\Lambda^{\text{hom}} = A\mathbb{Z}^3$. The reference configuration for the defect is a set $\Lambda \in \mathbb{R}^3$ satisfying

(RC) $\exists\, R_{\text{def}} > 0$, such that $\Lambda \backslash B_{R_{\text{def}}} = \Lambda^{\text{hom}} \backslash B_{R_{\text{def}}}$ and $\Lambda \cap B_{R_{\text{def}}}$ is finite.

For any $\ell \in \Lambda$, we define the set of its nearest neighbours:

$$\mathscr{N}(\ell) := \Big\{ m \in \Lambda \setminus \{\ell\} \,\Big|\, \exists\, x \in \mathbb{R}^3 \text{ s.t. } |x-\ell| = |x-m| \leq |x-k| \quad \forall\, k \in \Lambda \Big\}.$$

We remark that without loss of generality for $\Lambda = A\mathbb{Z}^3$ and for all $\ell \in \Lambda$, $\mathscr{N}(\ell) \supseteq \{\ell \pm Ae_i\}$ with $1 \leq i \leq 3$. If this fails for $A\mathbb{Z}^3$, there exists $A' \in \mathbb{R}^{3\times 3}$ satisfying $\Lambda = A\mathbb{Z}^3 = A'\mathbb{Z}^3$ and for all $\ell \in \Lambda$, $\mathscr{N}(\ell) \supseteq \{\ell \pm A'e_i\}$. Denote $\Lambda \setminus \ell = \Lambda \setminus \{\ell\}$, $\Lambda - \ell = \{m - \ell \,|\, m \in \Lambda \setminus \{\ell\}\}$ and $\Lambda^{\text{hom}}_* = \Lambda^{\text{hom}} \setminus \{0\}$. For $\ell \in \Lambda$, we define the following finite difference

$$D_\rho U(\ell) := U(\ell+\rho) - U(\ell) \qquad \text{for } U : \Lambda \to \mathbb{R}^3 \text{ and } \rho \in \Lambda - \ell \tag{6.1}$$

and $DU(\ell) := \{D_\rho U(\ell)\}_{\rho \in \Lambda - \ell}$. We consider $DU(\ell) \in (\mathbb{R}^3)^{\Lambda - \ell}$ to be a finite-difference stencil with infinite range. Let $\mathscr{N}(\ell) - \ell = \{m - \ell | m \in \mathscr{N}(\ell)\}$, then for any stencil $DU(\ell)$, define the norm

$$\begin{aligned} \big|DU(\ell)\big|_{\mathscr{N}} &:= \Big(\sum_{\rho \in \mathscr{N}(\ell)-\ell} \big|D_\rho U(\ell)\big|^2 \Big)^{1/2} \quad \text{and} \\ \|DU\|_{\ell^2(\Lambda)} &:= \Big(\sum_{\ell \in \Lambda} |DU(\ell)|^2_{\mathscr{N}} \Big)^{1/2} \end{aligned} \tag{6.2}$$

and the corresponding function space of finite-energy displacements

$$\dot{\mathscr{W}}^{1,2}(\Lambda) := \big\{ U : \Lambda \to \mathbb{R}^3 \,\big|\, \|DU\|_{\ell^2(\Lambda)} < \infty \big\}.$$

We also require the following subspace of compact displacements

$$\dot{\mathscr{W}}^{\text{c}}(\Lambda) := \big\{ U : \Lambda \to \mathbb{R}^3 \,\big|\, \exists\, R > 0 \text{ s.t. } U = \text{const in } \Lambda \setminus B_R \big\}.$$

We define $\dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})$ and $\dot{\mathscr{W}}^{\mathrm{c}}(\Lambda^{\mathrm{hom}})$ analogously.

Lemma 6.1. *Denote $\Lambda^1 = \Lambda, \Lambda^2 = \Lambda^{\mathrm{hom}}$, then for $i = 1, 2$, $\dot{\mathscr{W}}^{1,2}(\Lambda^i)$ is the closure of $\dot{\mathscr{W}}^{\mathrm{c}}(\Lambda^i)$ with respect to the norm $\|D \cdot \|_{\ell^2(\Lambda^i)}$.*

Proof of Lemma 6.1. This follows from [54, Proposition 9]. □

Define the reference deformation $Y_0 : \Lambda \to \mathbb{R}^3$ by $Y_0(\ell) = \ell$, then the space of admissible lattice deformations is defined as

$$\mathscr{A}(\Lambda) := \left\{ Y : \Lambda \to \mathbb{R}^3 |\, Y - Y_0 \in \dot{\mathscr{W}}^{1,2}(\Lambda) \right\}.$$

We define $U = Y - Y_0$ and refer to it as the displacement corresponding to Y. Given $Y \in \mathscr{A}(\Lambda)$ and $\ell, m \in \Lambda$, define

$$r_{\ell m} = r_{\ell m}(Y) = |Y(\ell) - Y(m)|.$$

Similarly, for Λ^{hom} we first define $Y_0^{\mathrm{hom}} : \Lambda^{\mathrm{hom}} \to \mathbb{R}^3$ by $Y_0^{\mathrm{hom}}(\ell) = \ell$ and the space of admissible lattice deformations as

$$\mathscr{A}(\Lambda^{\mathrm{hom}}) := \left\{ Y : \Lambda^{\mathrm{hom}} \to \mathbb{R}^3 |\, Y - Y_0^{\mathrm{hom}} \in \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}}) \right\}.$$

In order to utilise the uniformity of the locality estimates shown in Chapter 5, we introduce the following spaces, for $\lambda > 0$

$$\begin{aligned} \mathscr{A}(\Lambda, \lambda) &:= \left\{ Y : \Lambda \to \mathbb{R}^3 |\, \|D(Y - Y_0)\|_{\ell^2(\Lambda)} < \lambda \right\}, \\ \mathscr{A}(\Lambda^{\mathrm{hom}}, \lambda) &:= \left\{ Y : \Lambda^{\mathrm{hom}} \to \mathbb{R}^3 |\, \|D(Y - Y_0^{\mathrm{hom}})\|_{\ell^2(\Lambda^{\mathrm{hom}})} < \lambda \right\}. \end{aligned}$$

We also define the spaces of displacements corresponding to $\mathscr{A}(\Lambda, \lambda)$, $\mathscr{A}(\Lambda^{\mathrm{hom}}, \lambda)$. For $\lambda > 0$, define

$$\begin{aligned} \dot{\mathscr{W}}^{1,2}(\Lambda, \lambda) &:= \left\{ U \in \dot{\mathscr{W}}^{1,2}(\Lambda) \,\middle|\, \|DU\|_{\ell^2(\Lambda)} < \lambda \right\}, \\ \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}}, \lambda) &:= \left\{ U^{\mathrm{hom}} \in \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}}) \,\middle|\, \|DU^{\mathrm{hom}}\|_{\ell^2(\Lambda^{\mathrm{hom}})} < \lambda \right\}. \end{aligned}$$

It follows that

$$\mathscr{A}(\Lambda, \lambda) = Y_0 + \dot{\mathscr{W}}^{1,2}(\Lambda, \lambda) \quad \text{and} \quad \mathscr{A}(\Lambda^{\mathrm{hom}}, \lambda) = Y_0^{\mathrm{hom}} + \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}}, \lambda).$$

6.2 Site energy

Recall, in Chapter 5 the site energies were defined for nuclear configurations $Y \in \mathcal{Y}_{L^2}(M,\omega)$, which ensures that a unique TFW ground state corresponding to $m = m_Y \in \mathcal{M}_{L^2}(M,\omega)$ exists. The following result shows that the spaces $\mathscr{A}(\Lambda), \mathscr{A}(\Lambda^{\mathrm{hom}})$ and $\mathcal{Y}_{L^2}(M,\omega)$ are compatible.

Let $\eta \in C_{\mathrm{c}}^{\infty}(B_{R_0}(0))$ be radially symmetric function satisfying $\eta \geq 0$ and $\int_{\mathbb{R}^3} \eta = 1$ describe the charge density of a single (smeared) nucleus, for some fixed $R_0 > 0$. For any $Y \in \mathscr{A}(\Lambda)$ and $Y^{\mathrm{hom}} \in \mathscr{A}(\Lambda^{\mathrm{hom}})$, define the corresponding nuclear configurations

$$m_Y(x) = \sum_{\ell \in \Lambda} \eta(x - Y(\ell)), \qquad m_{Y^{\mathrm{hom}}}(x) = \sum_{\ell \in \Lambda^{\mathrm{hom}}} \eta(x - Y^{\mathrm{hom}}(\ell)). \tag{6.3}$$

Lemma 6.2. *Let $Y \in \mathscr{A}(\Lambda,\lambda) \cup \mathscr{A}(\Lambda^{\mathrm{hom}},\lambda)$, then there exist $M, \omega_0, \omega_1 > 0$, depending only on λ, such that m_Y defined in (6.3) satisfies $m_Y \in \mathcal{M}_{L^2}(M,\omega)$, where $\omega = (\omega_0, \omega_1)$.*

The uniformity of the constants M, ω_0, ω_1 appearing in Lemma 6.2 ensures that the locality estimates shown in Chapter 5 are also uniform for all $Y \in \mathscr{A}(\Lambda,\lambda) \cup \mathscr{A}(\Lambda^{\mathrm{hom}},\lambda)$.

In order to treat the lattice relaxation problem, we require site energies that are robust for large deformations. For this purpose, in this chapter, we construct site energies using the following family of partition functions, using the canonical construction described in Remark 12 in Chapter 5.

Choose $0 < \widetilde{\gamma} < \gamma$ and define $\widetilde{\varphi}(x) = e^{-\gamma|x|^2}$. Observe that $\widetilde{\varphi} \in C^{\infty}(\mathbb{R}^3)$, $\widetilde{\varphi} \geq 0$, is radially symmetric and satisfies

$$|\nabla^j \widetilde{\varphi}(x)| \leq C_j e^{-\widetilde{\gamma}|x|}, \quad \text{for all } j \in \mathbb{N}. \tag{6.4}$$

Given $Y \in \mathscr{A}(\Lambda,\lambda)$, recall (5.2), that there exists $R' = R'(\lambda) > 0$ such that $\cup_{\ell \in \Lambda} B_{R'}(Y(\ell)) = \mathbb{R}^3$. Then, for $\ell \in \Lambda$, define

$$\varphi_\ell(Y;x) = \frac{\widetilde{\varphi}(x - Y(\ell))}{\sum_{\ell' \in \Lambda} \widetilde{\varphi}(x - Y(\ell'))}. \tag{6.5}$$

This is finite as $\sum_{\ell' \in \Lambda} \widetilde{\varphi}(x - Y(\ell')) \geq e^{-\gamma(R')^2} > 0$ for all $x \in \mathbb{R}^3$. Moreover, this construction satisfies (5.6) and (5.84) for all $k \in \mathbb{N}$. Similarly, for $Y^{\text{hom}} \in \mathscr{A}(\Lambda^{\text{hom}}, \lambda)$ and $\ell \in \Lambda^{\text{hom}}$, we define

$$\varphi_\ell(Y^{\text{hom}}; x) = \frac{\widetilde{\varphi}(x - Y^{\text{hom}}(\ell))}{\sum_{\ell' \in \Lambda^{\text{hom}}} \widetilde{\varphi}(x - Y^{\text{hom}}(\ell'))}.$$

Now, for $Y \in \mathscr{A}(\Lambda, \lambda)$, $Y^{\text{hom}} \in \mathscr{A}(\Lambda^{\text{hom}}, \lambda)$ recall the energy densities $\mathcal{E}_1(Y; \cdot)$, $\mathcal{E}_1(Y^{\text{hom}}; \cdot)$ defined in (5.4). For $\ell_1 \in \Lambda$, $\ell_2 \in \Lambda^{\text{hom}}$, define $E_{\ell_1} : \mathscr{A}(\Lambda) \to \mathbb{R}$ and $E_{\ell_2} : \mathscr{A}(\Lambda^{\text{hom}}) \to \mathbb{R}$ by

$$E_{\ell_1}(Y) := \int_{\mathbb{R}^3} \mathcal{E}_1(Y; x)\, \varphi_{\ell_1}(Y; x)\, \mathrm{d}x, \tag{6.6}$$

$$E_{\ell_2}(Y^{\text{hom}}) := \int_{\mathbb{R}^3} \mathcal{E}_1(Y^{\text{hom}}; x)\, \varphi_{\ell_2}(Y^{\text{hom}}; x)\, \mathrm{d}x. \tag{6.7}$$

Remark 19. The definition of the site energies (6.6)–(6.7) are equivalent to the definition (5.7) given in Chapter 5. The only distinction is that in (5.7) the nuclear coordinates are indexed using $\mathbb{N}$, whereas (6.6)–(6.7) use Λ and Λ^{hom}, respectively. As **(RC)** implies that $\Lambda, \Lambda^{\text{hom}}$ are countable, hence there exist bijections that exchange the indices.

Recall that in (5.4)–(5.5), we defined two energy densities $\mathcal{E}_1(Y; \cdot)$, $\mathcal{E}_2(Y; \cdot)$ corresponding to $Y \in \mathcal{Y}_{L^2}(M, \omega)$. Alternatively, one could equivalently use $\mathcal{E}_2(Y; \cdot)$ to define the site energies (6.6)–(6.7) for the lattice relaxation problem and the entire analysis would hold, though some proofs would require some minor changes. $\square$

The following result collects the properties of the site energies. The locality properties and invariance of the site energies under isometries and permutations have been explored in detail in Chapter 5. However, we also establish an additional property, which we refer to as homogeneity of the site energies, that we now discuss.

Suppose two deformations Y_1, Y_2 possess sites ℓ_1, ℓ_2 whose nuclear configurations agree in a finite region. The homogeneity result controls the difference between the site energies $E_{\ell_1}(Y_1)$ and $E_{\ell_2}(Y_2)$, depending on the size of the agreement region. Consequently, the homogeneity result demonstrates the dependence of the site energies on the surrounding nuclear arrangement.

Without accounting for lattice relaxation, a point defect introduces a local perturbation to the crystal. As a result, sufficiently far from the defect core, the defective lattice becomes indistinguishable from the unperturbed arrangement. The homogeneity estimate will be used to show that the site energy inherits this property, so the difference between the defective site energy and the homogeneous site energy is negligible far from the defect core. This allows us to exploit the symmetry properties of the perfect crystal when treating the relaxation of a defective crystal.

Proposition 6.3. *The site energies* $\{E_\ell\}_{\ell\in\Lambda}, \{E_\ell\}_{\ell\in\Lambda^{\rm hom}}$ *defined in* (6.6)–(6.7) *satisfy* **(SE)***:*

Let $Y \in \mathscr{A}(\Lambda,\lambda) \cup \mathscr{A}(\Lambda^{\rm hom},\lambda)$ *and let* $\Lambda' = \mathrm{Dom}(Y)$ *denote the domain of* Y*.*

(SE.R) *Regularity: At each* $\ell \in \Lambda'$*,* $E_\ell(Y)$ *possesses all partial derivatives, denoted by* $E_{\ell,\mathbf{n}}(Y)$*,* $\mathbf{n} \in (\Lambda' \setminus \ell)^j$ *for* $j \in \mathbb{N}$*.*

(SE.L) *Locality: There exists* $\gamma > 0$ *such that for all* $j \in \mathbb{N}$ *and* $\ell \in \Lambda$*,* $\mathbf{n} \in (\Lambda \setminus \ell)^j$

$$|E_{\ell,\mathbf{n}}(Y)| \le C_j e^{-\gamma\sum_{i=1}^{j} r_{\ell n_i}},$$

where $C_j = C_j(\lambda), \gamma = \gamma(\lambda)$ *and* $r_{\ell n_i} = |Y(\ell) - Y(n_i)|$*.*

(SE.H) *Homogeneity: Let* $Y_1, Y_2 \in \mathscr{A}(\Lambda,\lambda) \cup \mathscr{A}(\Lambda^{\rm hom},\lambda)$ *and for* $i = 1, 2$*, let* $\Lambda'_i = \mathrm{Dom}(Y_i)$*. There exist* $C = C(\lambda), \gamma = \gamma(\lambda) > 0$ *such that for any* $\ell_1 \in \Lambda'_1, \ell_2 \in \Lambda'_2$ *and* $r \ge 0$ *satisfying*

$$\begin{aligned} &\{Y_1(n_1) - Y_1(\ell_1) \mid n_1 \in \Lambda'_1 \ \textit{s.t.}\ r_{\ell_1 n_1}(Y_1) \le r\} \\ &= \{Y_2(n_2) - Y_2(\ell_2) \mid n_2 \in \Lambda'_2 \ \textit{s.t.}\ r_{\ell_2 n_2}(Y_2) \le r\}, \end{aligned} \tag{6.8}$$

then

$$|E_{\ell_1}(Y_1) - E_{\ell_2}(Y_2)| \le Ce^{-\gamma r}.$$

Additionally, for any $n_1 \in \Lambda'_1 \setminus \ell_1$ *satisfying* $r_{\ell_1 n_1}(Y_1) \le r$*, we have*

$$|E_{\ell_1,n_1}(Y_1) - E_{\ell_2,n_2}(Y_2)| \le Ce^{-\gamma(r + r_{\ell_1 n_1})},$$

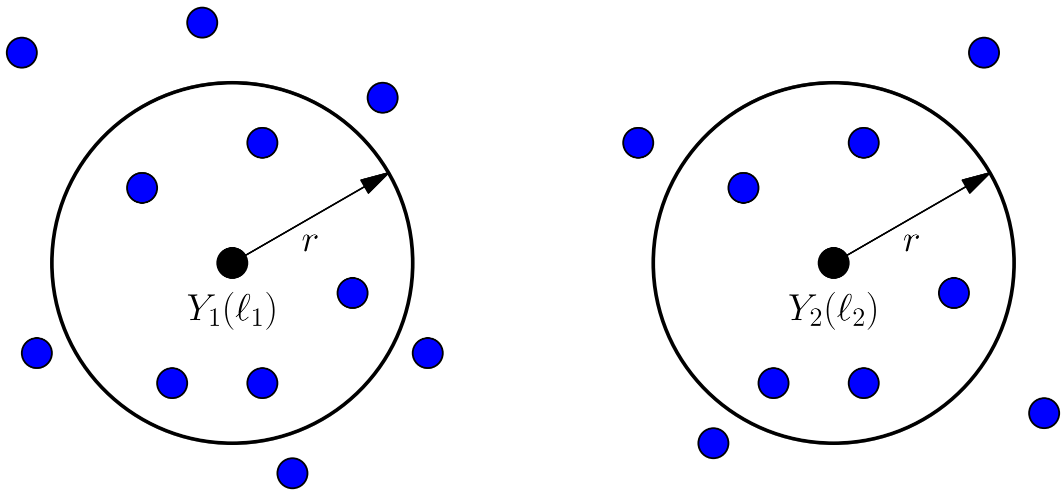


Figure 6.1: A diagram showing the assumption (6.8) appearing in **(SE.H)**.

where n_2 is the unique element of $\Lambda_2' \setminus \ell_2$ satisfying
$Y_1(n_1) - Y_1(\ell_1) = Y_2(n_2) - Y_2(\ell_2)$.

(SE.P) *Symmetry under permutations: If $\pi : \Lambda' \to \Lambda'$ is a bijection, then $Y \circ \pi \in \mathscr{A}(\Lambda', \lambda)$ and $E_{\pi(\ell)}(Y \circ \pi) = E_\ell(Y)$.*

(SE.I) *Symmetry under isometries: If $\varphi : \mathbb{R}^3 \to \mathbb{R}^3$ is an isometry, then $\varphi \circ Y \in \mathscr{A}(\Lambda', \lambda)$ and $E_\ell(\varphi \circ Y) = E_\ell(Y)$.*

Remark 20. Though the locality and homogeneity estimates **(SE.L)** and **(SE.H)** appear similar, logically one does not imply the other. However, their similarity arises as both results are consequences of the locality estimates established in Chapter 3.

Remark 21. Homogeneity and permutation invariance imply that all atoms in the system are of the same species. One could extend the assumptions to admit multiple species of atoms, however the generalisation will bring significantly more complex notations and we will not pursue them here. □

6.3 Site potential

The property **(SE.I)** implies that the site energies are translation invariant, hence

$$E_\ell(Y) = E_\ell(Y - Y(\ell)) \qquad \forall\, Y \in \mathscr{A}(\Lambda), \ell \in \Lambda. \tag{6.9}$$

It follows from (6.9) that $E_\ell(Y)$ is only a function of $DY(\ell)$, and hence a function of $DU(\ell)$.

For $\ell_1 \in \Lambda$ and $\ell_2 \in \Lambda^{\mathrm{hom}}$, define the spaces

$$\begin{aligned} D_{\ell_1}(\Lambda) &:= \big\{ DU(\ell_1) \,\big|\, U \in \dot{\mathscr{W}}^{1,2}(\Lambda) \big\} \subset (\mathbb{R}^3)^{\Lambda - \ell_1}, \\ D_{\ell_2}(\Lambda^{\mathrm{hom}}) &:= \big\{ DU^{\mathrm{hom}}(\ell_2) \,\big|\, U^{\mathrm{hom}} \in \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}}) \big\} \subset (\mathbb{R}^3)^{\Lambda_*^{\mathrm{hom}}}. \end{aligned}$$

Due to the translation-invariance of Λ^{hom}, it follows that $D_\ell(\Lambda^{\mathrm{hom}}) = D_m(\Lambda^{\mathrm{hom}})$ for all $\ell, m \in \Lambda^{\mathrm{hom}}$, hence we define the space $D(\Lambda^{\mathrm{hom}}) := D_\ell(\Lambda^{\mathrm{hom}})$ for all $\ell \in \Lambda^{\mathrm{hom}}$.

For $\ell \in \Lambda$, define the site potential $V_\ell : D_\ell(\Lambda) \to \mathbb{R}$ by

$$V_\ell\big(DU(\ell)\big) := E_\ell(Y_0 + U). \tag{6.10}$$

Similarly, for $\ell \in \Lambda^{\mathrm{hom}}$, define $V_\ell^{\mathrm{hom}} : D(\Lambda^{\mathrm{hom}}) \to \mathbb{R}$ by

$$V_\ell^{\mathrm{hom}}\big(DU^{\mathrm{hom}}(\ell)\big) := E_\ell(Y_0^{\mathrm{hom}} + U^{\mathrm{hom}}). \tag{6.11}$$

It follows from **(SE.P)** that $V_{\ell_1}^{\mathrm{hom}} = V_{\ell_2}^{\mathrm{hom}}$ for all $\ell_1, \ell_2 \in \Lambda^{\mathrm{hom}}$, hence there exists a homogeneous site potential $V^{\mathrm{hom}} : D(\Lambda^{\mathrm{hom}}) \to \mathbb{R}$ satisfying

$$V^{\mathrm{hom}}\big(DU^{\mathrm{hom}}(\ell)\big) = E_\ell(Y_0^{\mathrm{hom}} + U^{\mathrm{hom}}) \tag{6.12}$$

for all $U \in \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})$ and $\ell \in \Lambda^{\mathrm{hom}}$. We now justify this claim.

Let $\ell, m \in \Lambda^{\mathrm{hom}}$ and $U^{\mathrm{hom}} \in \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})$, then define $Y = Y_0^{\mathrm{hom}} + U^{\mathrm{hom}}$. Now define a bijection $\pi : \Lambda^{\mathrm{hom}} \to \Lambda^{\mathrm{hom}}$ by $\pi(k) = k + \ell - m$ and let $U_1^{\mathrm{hom}} := U^{\mathrm{hom}} \circ \pi$ and $Y_1 := Y \circ \pi = Y_0^{\mathrm{hom}} \circ \pi + U_1^{\mathrm{hom}}$. It follows from the definition that $DU_1^{\mathrm{hom}}(m) = DU^{\mathrm{hom}}(\ell)$. By applying **(SE.P)** to (6.11), we deduce

$$\begin{aligned} V_\ell^{\mathrm{hom}}\big(DU^{\mathrm{hom}}(\ell)\big) &= E_\ell(Y_0^{\mathrm{hom}} + U^{\mathrm{hom}}) = E_m(Y_1) \\ &= V_m^{\mathrm{hom}}\big(DU_1^{\mathrm{hom}}(m)\big) = V_m^{\mathrm{hom}}\big(DU^{\mathrm{hom}}(\ell)\big), \end{aligned}$$

hence V_ℓ^{hom} is independent of $\ell \in \Lambda^{\mathrm{hom}}$, so we refer to the function as V^{hom}.

From the definitions (6.10)–(6.12), it is clear that the site potentials inherit the regularity, locality and homogeneity properties satisfied by the site energies. The full statement of the properties of the site potentials is given in Theorem 6.14 on Page 189.

Remark 22. The key distinction between the site energy $E_\ell(Y_0 + U)$ and the site potential $V_\ell(DU(\ell))$ is that calculating the derivative $\langle E_{\ell,n}(Y_0 + U), V\rangle$ involves evaluating $V(n)$. In contrast, the derivative $\langle V_{\ell,n}(DU(\ell)), V\rangle$ can be evaluated using $DV(n)$, which can be estimated by the norm $\|DV\|_{\ell^2(\Lambda)}$.

This exposes the finite-difference structure of the site energies, and allows us to control the energy of an arrangement using the gradients of a displacement and not the displacement itself. □

6.4 Energy difference functionals

Using the site potentials $\{V_\ell\}_{\ell\in\Lambda}$, we formally define the energy-difference functional for a displacement $U \in \dot{\mathscr{W}}^{1,2}(\Lambda)$:

$$\mathscr{E}(U) := \sum_{\ell\in\Lambda} \Big(E_\ell(Y_0 + U) - E_\ell(Y_0)\Big) = \sum_{\ell\in\Lambda} \Big(V_\ell\big(DU(\ell)\big) - V_\ell\big(0\big)\Big).$$

Similarly, for $U^{\mathrm{hom}} \in \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})$, we also formally define

$$\begin{aligned} \mathscr{E}^{\mathrm{hom}}(U^{\mathrm{hom}}) &:= \sum_{\ell\in\Lambda^{\mathrm{hom}}} \Big(E_\ell(Y_0^{\mathrm{hom}} + U^{\mathrm{hom}}) - E_\ell(Y_0^{\mathrm{hom}})\Big) \\ &= \sum_{\ell\in\Lambda^{\mathrm{hom}}} \Big(V^{\mathrm{hom}}\big(DU^{\mathrm{hom}}(\ell)\big) - V^{\mathrm{hom}}\big(0\big)\Big). \end{aligned}$$

The argument presented in Remark 22 ensures that the energy difference functionals $\mathcal{E}$ and $\mathcal{E}^{\mathrm{hom}}$ are defined on $\dot{\mathscr{W}}^{1,2}(\Lambda)$ and $\dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})$, respectively.

Theorem 6.4. *Denote $\Lambda_1 = \Lambda, \Lambda_2 = \Lambda^{\rm hom}$ and $\mathscr{E}_1 = \mathscr{E}, \mathscr{E}_2 = \mathscr{E}^{\rm hom}$.*

For $i = 1, 2$, $\mathscr{E}_i : \dot{\mathscr{W}}^{\rm c}(\Lambda_i) \to \mathbb{R}$ is continuous with respect to $\|D\cdot\|_{\ell^2(\Lambda_i)}$, hence there exists a unique continuous extension to $\dot{\mathscr{W}}^{1,2}(\Lambda_i)$, which we denote by $\mathscr{E}_i$. The extended functional $\mathscr{E}_i : \dot{\mathscr{W}}^{1,2}(\Lambda_i) \to \mathbb{R}$ is twice continuously differentiable.

The homogeneous energy $\mathscr{E}^{\rm hom}$ is used in the analysis in order to show that $\mathscr{E}$ is well-defined on $\dot{\mathscr{W}}^{1,2}(\Lambda)$. A key step in the proof of Theorem 6.4 involves proving that $\delta\mathscr{E}(0)$ defines a bounded functional on $\dot{\mathscr{W}}^{\rm c}(\Lambda)$. On the homogeneous lattice $\delta\mathscr{E}^{\rm hom}(0) = 0$ holds due to the symmetries of the perfect lattice $\Lambda^{\rm hom}$. By applying the homogeneity estimates established in **(SE.H)**, we then establish that $\delta\mathscr{E}(0) = \delta\mathscr{E}(0) - \delta\mathscr{E}^{\rm hom}(0)$ is a well-defined operator acting on $\dot{\mathscr{W}}^{\rm c}(\Lambda)$.

Once this has been established, for $U \in \dot{\mathscr{W}}^{\rm c}(\Lambda)$ we can express

$$\mathscr{E}(U) - \mathscr{E}(0) = \Big(\mathscr{E}(U) - \mathscr{E}(0) - \langle \mathscr{E}(0), U\rangle\Big) + \langle \mathscr{E}(0), U\rangle.$$

The term appearing the right hand side can then be controlled in terms of $\|DU\|^2_{\ell^2(\Lambda)}$ by applying the locality estimates **(SE.L)**.

This argument requires an equivalent norm that uses an exponentially-weighted finite difference, which we define in Section 6.6.2, instead of the nearest-neighbour norm (6.2). The proof is presented in detail in Section 6.9.

6.5 Variational problem for point defects

We establish Theorem 6.4 for the sole purpose of formulating the variational problem

$$\text{Find } \bar{U} \in \arg\min\big\{\mathscr{E}(U) \,\big|\, U \in \dot{\mathscr{W}}^{1,2}(\Lambda)\big\}, \tag{6.13}$$

where "arg min" is understood in the sense of local minimality. We may also consider the minimisation problem over the restricted space $\dot{\mathscr{W}}^{1,2}(\Lambda, \lambda)$, for $\lambda > 0$

$$\text{Find } \bar{U} \in \arg\min\big\{\mathscr{E}(U) \,\big|\, U \in \dot{\mathscr{W}}^{1,2}(\Lambda, \lambda)\big\}. \tag{6.14}$$

It follows that any minimiser to (6.13) is also a minimiser to (6.14), provided $\lambda > 0$ is sufficiently large.

We shall only be concerned with the structure of solutions to (6.14), *assuming* their existence.

Remark 23. A standard argument to prove the existence of minimisers of a functional is to use convexity properties to prove the lower semi continuity of the functional. We recall that for a fixed finite nuclear arrangement, the TFW energy $E^{\mathrm{TFW}}(\sqrt{\rho}, m)$, defined in (1.1), is strictly convex with respect to the electron density term $\sqrt{\rho}$. However, the permutation invariance property **(SE.P)** implies that $\mathscr{E}$ is not convex.

Additionally, due to the permutation invariance property **(SE.P)**, any nuclear arrangement that minimises $\mathscr{E}$ could be described by many lattice displacements. It follows that physically many minimisers of (6.14) should exist. However, as the parameter $\lambda > 0$ controls the size of the test space $\dot{\mathscr{W}}^{1,2}(\Lambda, \lambda)$, altering λ would likely change the number of solutions to (6.14). $\square$

If $\bar{U}$ solves (6.14), then $\bar{U}$ is a second-order critical point, satisfying

$$\langle \delta\mathscr{E}(\bar{U}), V \rangle = 0 \qquad \text{and} \qquad \langle \delta^2\mathscr{E}(\bar{U})V, V \rangle \geq 0 \qquad \forall\, V \in \dot{\mathscr{W}}^{1,2}(\Lambda). \quad (6.15)$$

We now establish the rate of decay for minimising displacements. To show this, we require the following strong stability condition for the host homogeneous lattice.

(LS) *Lattice stability:* There exists $c_{\mathrm{L}} > 0$ depending only on Λ^{hom}, such that

$$\big\langle \delta^2\mathscr{E}^{\mathrm{hom}}(0)V, V \big\rangle \geq c_{\mathrm{L}} \|DV\|^2_{\ell^2(\Lambda^{\mathrm{hom}})} \qquad \forall\, V \in \dot{\mathscr{W}}^{\mathrm{c}}(\Lambda^{\mathrm{hom}}). \qquad (6.16)$$

As $\delta\mathscr{E}^{\mathrm{hom}}(0) = 0$, this stability condition states that the equilibrium configuration $U^{\mathrm{hom}} \equiv 0$ is a local minimiser for $\mathscr{E}^{\mathrm{hom}}$.

Theorem 6.5. *If* **(LS)** *is satisfied, then for any $\bar{U}$ solving* (6.14) *there exist $C = C(\lambda) > 0$ and $\bar{U} \in \mathbb{R}^3$ such that for all $\ell \in \Lambda \setminus B_{R_{\mathrm{def}}}$*

$$|\bar{U}(\ell) - \bar{U}_\infty| \leq C\big(1 + |\ell|\big)^{-2}. \qquad (6.17)$$

In addition, for all $\ell \in \Lambda \setminus B_{R_{\rm def}}$ and $\rho \in \Lambda - \ell$

$$|\rho|^{-1}\big|D_\rho \bar{U}(\ell)\big| \leq C\big(1+|\ell|\big)^{-3}. \tag{6.18}$$

Numerical experiments performed in [23, Section 2.7] confirm the sharpness of the decay results presented in Theorem 6.5 for models with finite-range interaction.

We prove Theorem 6.5 by adapting the proof of [23, Theorem 2.3]. This argument requires the Green's function for the homogeneous lattice $\Lambda^{\rm hom}$, whose definition relies on the stability condition **(LS)**.

The remainder of this chapter is dedicated to proving our main results.

6.6 Preliminary results

We now collect some technical lemmas that will be used in the proof of our main results.

6.6.1 Path counting lemmas

The following section contains two technical lemmas that will be used throughout this chapter.

Lemma 6.6. *For all $\ell \in \Lambda$ and $\rho \in \Lambda - \ell$, there exists a finite path of lattice points $\mathscr{P}(\ell, \ell+\rho) := \{\ell_i\}_{1 \leq i \leq N_\rho + 1} \subset \Lambda$, such that for each $1 \leq i \leq N_\rho$, $\ell_{i+1} \in \mathscr{N}(\ell_i)$. Moreover, there exists $C_0 > 0$, independent of ℓ and ρ, such that $N_\rho \leq C_0|\rho|$.*

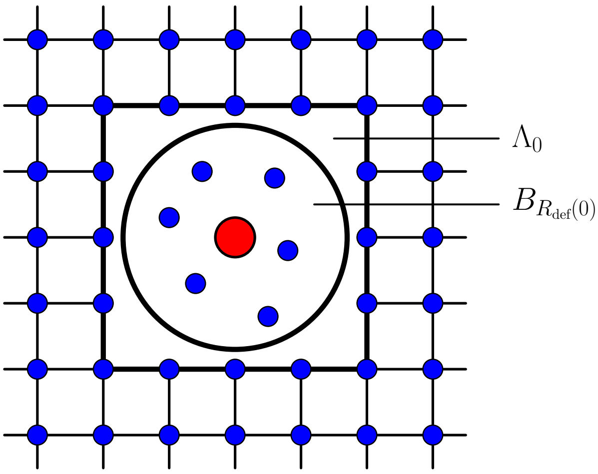
Lemma 6.7. *For $\ell \in \Lambda$ and $n \in \mathbb{N}$, define*

$$\mathscr{B}_n(\ell) = \left\{(\ell_1,\ell_2) \in \Lambda^2 \,\middle|\, n-1 < |\ell_1 - \ell_2| \leq n, \ell \in \mathscr{P}(\ell_1,\ell_2)\right\},$$

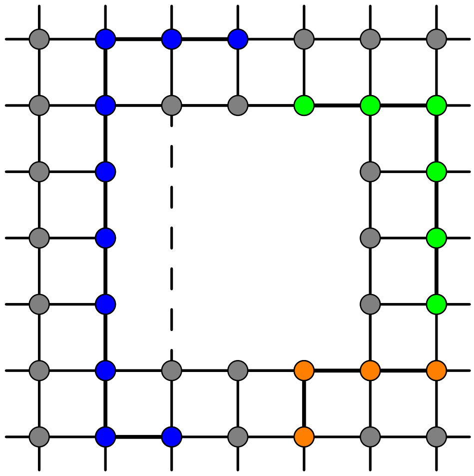
then there exists $C > 0$ such that

$$|\mathscr{B}_n(\ell)| \leq Cn^6 \quad \textit{for all } \ell \in \Lambda. \tag{6.19}$$

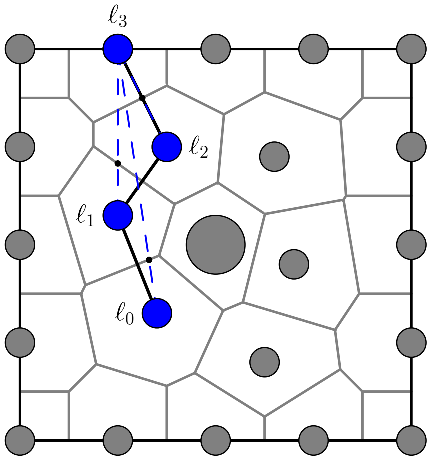
We remark that these results are fairly obvious from a geometrical viewpoint, but the proofs are included below for completeness.



(a) The construction of Λ_0.



(b) Examples of paths constructed outside of Λ_0, using the perfect lattice Λ^{hom}.



(c) A diagram showing the construction of a path inside Λ_0. This involves decomposing Λ_0 using Voronoi cells, whose boundaries are coloured grey.

Figure 6.2: Diagrams represented the arguments used to prove Lemmas 6.6 and 6.7.

Proof of Lemma 6.6. Let $\Gamma \subset \mathbb{R}^3$ denote the unit cell of the lattice Λ^{hom}, centred at 0. This is also referred to as the Wigner–Seitz cell or Voronoi cell of Λ^{hom}, which is a semi-open subset of $\mathbb{R}^3$ that contains all points in $\mathbb{R}^3$ that are closer to $0 \in \Lambda^{\mathrm{hom}}$ than all other points in Λ^{hom} and also satisfies

$$\bigcup_{\ell \in \Lambda^{\mathrm{hom}}} (\Gamma + \ell) = \mathbb{R}^3,$$

where $\Gamma + \ell = \{\, x + \ell \,|\, x \in \Gamma \,\}$. By the definition of Γ, there exists $\delta > 0$ such that $B_\delta(0) \subset \Gamma$, hence choosing $k = \lceil \frac{R_{\mathrm{def}}}{\delta} \rceil \in \mathbb{N}$ ensures that $B_{R_{\mathrm{def}}}(0) \subset k\Gamma$. Then define $\Lambda_0 = \Lambda \cap k\bar{\Gamma}$, which satisfies: Λ_0 is finite, $\Lambda_0^c := \Lambda \setminus \Lambda_0 = \Lambda^{\mathrm{hom}} \setminus \Lambda_0$ and $\partial\Lambda_0 \subset \Lambda^{\mathrm{hom}}$.

Case 1 First consider $\ell \in (\Lambda_0^c \cup \partial\Lambda_0), \rho \in (\Lambda_0^c \cup \partial\Lambda_0) - \ell$, then $\rho \in \Lambda^{\mathrm{hom}}$ and can be expressed as $\rho = \sum_{j=1}^3 n_j A e_j$, where $(Ae_j)_{1 \le j \le 3}$ are the lattice vectors and $(n_j) \in \mathbb{Z}^3$. As the lattice vectors are independent, one can define the norm $|\rho|_1 = \sum_{j=1}^3 |n_j|$, which is equivalent to the standard norm $|\rho|$, hence $|\rho|_1 \le C|\rho|$.

It is straightforward to construct a lattice path $(\ell_i)_{1 \le i \le N_\rho} \subset (\Lambda_0^c \cup \partial\Lambda_0)$, from ℓ to $\ell + \rho$, such that $\ell_{i+1} \in \{\ell_i \pm Ae_j\}_{1 \le j \le 3} \subseteq \mathscr{N}(\ell_i)$, such that
$N_\rho \le 2|\rho|_1 \le C|\rho|$.

Case 2 Now consider $\ell \in \Lambda_0, \rho \in \Lambda_0 - \ell$. For $\ell' \in \Lambda, \rho' \in \Lambda - \ell'$, then define the Voronoi cell $\mathcal{V}(\ell')$ and it's boundary $\partial\mathcal{V}(\ell')$ by

$$\begin{aligned} \mathcal{V}(\ell') &= \left\{ x \in \mathbb{R}^3 \,\middle|\, |x - \ell'| \le |x - k| \quad \forall\, k \in \Lambda \right\}, \\ \partial\mathcal{V}(\ell') &= \left\{ x \in \mathcal{V}(\ell') \,\middle|\, |x - \ell'| = |x - m| \text{ for some } m \in \mathscr{N}(\ell') \right\}. \end{aligned} \tag{6.20}$$

Also, define the function $d_{\ell'} : \mathbb{R}^3 \to \mathbb{R}_{\ge 0}$ by

$$d_{\ell'}(x) := \max_{k \in \Lambda \setminus \{\ell'\}} \left(|x - \ell'| - |x - k| \right).$$

By **(RC)**, there exists $\mu > 0$ such that $|\ell_1 - \ell_2| \ge \mu > 0$ for all $\ell_1, \ell_2 \in \Lambda$ such that $\ell_1 \ne \ell_2$. It follows that $d_{\ell'}$ is continuous and satisfies $d_{\ell'}(\ell') \le -\mu < 0$ and $d_{\ell'}(k) \ge \mu > 0$ for all $k \in \Lambda \setminus \{\ell'\}$. Moreover, it follows that $\mathcal{V}(\ell') = \{x | d_{\ell'}(x) \le 0\}$ and $\partial\mathcal{V}(\ell') = \{x | d_{\ell'}(x) = 0\}$. For $t \in [0, 1]$ define $f(t) = d_{\ell'}(\ell' + t\rho')$. As f is continuous and satisfies $f(0) < 0, f(1) > 0$, by the Intermediate Value

Theorem, there exists $t_0 \in (0,1)$ such that $f(t_0) = d_{\ell'}(\ell' + t_0\rho') = 0$, hence $\ell' + t_0\rho' \in \partial\mathcal{V}(\ell')$, hence there exists $m = m(\ell', \ell' + \rho') \in \mathscr{N}(\ell')$ such that $t_0|\rho'| = |\ell' + t_0\rho' - \ell'| = |\ell' + t_0\rho' - m|$. By the triangle inequality, it follows that

$$|\ell' + \rho' - m| \leq |\ell' + t_0\rho' - m| + |(1-t_0)\rho'| = t_0|\rho'| + (1-t_0)|\rho'| = |\rho'|. \tag{6.21}$$

We now show that the inequality in (6.21) is actually strict. Define the line $L = \{\ell' + t\rho' | t \in \mathbb{R}\}$ and the surface $S = \{x \in \mathbb{R}^3 | |x - \ell'| = |x - m|\}$. Observe that L and S can intersect at most once and $\ell' + t_0\rho' \in L \cap S$, where $t_0 \in (0,1)$. It follows that as $\ell' + \rho' \in L$, $\ell' + \rho' \notin S$ so (6.21) ensures that

$$|\ell' + \rho' - m| < |\rho'|. \tag{6.22}$$

We use (6.22) to construct a finite path of neighbouring lattice points from ℓ' to $\ell' + \rho'$. Let $\ell_1(\ell', \rho') = \ell'$, then for $i \in \mathbb{N}$, given $\ell_i(\ell', \rho')$, define $\ell_{i+1}(\ell', \rho') = m(\ell_i, \ell' + \rho') \in \mathscr{N}(\ell_i)$, which satisfies

$$|\ell' + \rho' - \ell_{i+1}| < |\ell' + \rho' - \ell_i|. \tag{6.23}$$

We now show that this path reaches $\ell' + \rho'$ after finitely many steps. Observe that $\ell_1 = \ell' \in \Lambda \cap B_{|\rho'|+1}(\ell' + \rho')$, which is a finite set. The estimate (6.23) implies that $\ell_2 \in \Lambda \cap B_{|\rho'|+1}(\ell' + \rho') \setminus \{\ell_1\}$, and arguing inductively it follows if $\ell_j \neq \ell' + \rho'$ for all $j \leq i$, then $\ell_{i+1} \in \Lambda \cap B_{|\rho'|+1}(\ell' + \rho') \setminus \{\ell_1, \dots, \ell_i\}$. Let $N = N_{\ell',\rho'} = |\Lambda \cap B_{|\rho'|+1}(\ell' + \rho')|$, and suppose that after $N-1$ steps, the path has not reached $\ell' + \rho'$, hence $\ell_N \in \Lambda \cap B_{|\rho'|+1}(\ell' + \rho') \setminus \{\ell_1, \dots, \ell_{N-1}\} = \{\ell' + \rho'\}$, hence there exists a finite path of neighbouring lattice points for any $\ell', \ell' + \rho'$.

Now consider the set

$$\{\ell_i(\ell, \rho) | \ell \in \Lambda_0, \rho \in \Lambda_0 - \ell, 1 \leq i \leq N_{\ell,\rho} - 1\},$$

which is finite, hence there exists $c_0 > 0$ such that: for all $\ell \in \Lambda_0, \rho \in \Lambda_0 - \ell$,

$1 \leq i \leq N_{\ell,\rho} - 1$, $\ell_i = \ell_i(\ell, \rho)$ and $\ell_{i+1} = \ell_{i+1}(\ell, \rho)$ satisfy

$$|\ell + \rho - \ell_{i+1}| \leq |\ell + \rho - \ell_i| - c_0.$$

As $\ell_1 = \ell$ satisfies $|\ell + \rho - \ell_1| = |\rho|$, by arguing inductively we deduce

$$|\ell + \rho - \ell_{i+1}| \leq |\rho| - c_0 i.$$

Observe that for $i \geq N_\rho := \lceil c_0^{-1} |\rho| \rceil$, $|\ell + \rho - \ell_{i+1}| \leq |\rho| - c_0 i \leq 0$, hence the path reaches $\ell + \rho$ within $N_\rho \leq c_0^{-1}|\rho| + 1 \leq (c_0^{-1} + \mu^{-1})|\rho| = C|\rho|$ steps.

Case 3 It remains to consider the case $\ell \in \Lambda_0 \setminus \partial\Lambda_0, \rho \in \Lambda_0^c \setminus \{\ell\}$, as the case $\ell \in \Lambda_0^c, \rho \in (\Lambda_0 \setminus \partial\Lambda_0) \setminus \{\ell\}$ can be treated identically. We follow the procedure of Case 2, starting from $\ell_1 = \ell$ and moving along neighbouring lattice points in Λ_0 until the boundary $\partial\Lambda_0$ is reached, hence there exist neighbouring lattice points $\ell_1, \ldots \ell_{i-1} \in \Lambda_0 \setminus \partial\Lambda_0$ and $\ell_i \in \partial\Lambda_0$ satisfying $|\ell + \rho - \ell_i| \leq |\rho| - c_0(i-1)$. As $\ell_i, \ell + \rho \in \Lambda_0^c \cup \partial\Lambda_0$, by Case 1, there exists a lattice path $(\ell'_j)_{1 \leq j \leq N_{i,\rho}} + 1$ along neighbouring lattice points, from ℓ_i to $\ell + \rho$, satisfying $N_{i,\rho} \leq C|\ell + \rho - \ell_i| \leq C\left(|\rho| - c_0(i-1)\right)$, hence joining these paths creates a lattice path of neighbouring points from ℓ to $\ell + \rho$ of length $N_\rho + 1$, where $N_\rho = i + N_{i,\rho} \leq C(c_0 i + N_{i,\rho}) \leq C|\rho|$. □

Proof of Lemma 6.7. Fix $\ell \in \Lambda$, $n \in \mathbb{N}$ and recall the subset $\Lambda_0 \subset \Lambda$ defined in the proof of Lemma 6.6. We estimate consider $|\mathscr{B}_n(\ell) \cap (\Lambda_0 \times \Lambda_0)|$. Since Λ_0 is finite, it follows that

$$|\mathscr{B}_n(\ell) \cap (\Lambda_0 \times \Lambda_0)| \leq |\Lambda_0 \times \Lambda_0| = |\Lambda_0|^2 \leq |\Lambda_0|^2 n^3. \tag{6.24}$$

Next, observe that

$$(\ell_1, \ell_2) \in \mathscr{B}_n(\ell) \cap (\Lambda_0 \times \Lambda_0^c) \quad \text{ if and only if } \quad (\ell_2, \ell_1) \in \mathscr{B}_n(\ell) \cap (\Lambda_0^c \times \Lambda_0),$$

hence $|\mathscr{B}_n(\ell) \cap (\Lambda_0 \times \Lambda_0^c)| = |\mathscr{B}_n(\ell) \cap (\Lambda_0^c \times \Lambda_0)|$. Also, if $(\ell_1, \ell_2) \in \mathscr{B}_n(\ell)$, then (6.23) implies $|\ell - \ell_2| < |\ell_1 - \ell_2| \leq n$, hence as $\Lambda_0^c = \Lambda^{\text{hom}} \setminus \Lambda_0$

$$\begin{aligned} |\mathscr{B}_n(\ell) \cap (\Lambda_0 \times \Lambda_0^c)| &\leq |\Lambda_0 \times (\Lambda^{\text{hom}} \cap B_n(\ell))| = |\Lambda_0||\Lambda^{\text{hom}} \cap B_n(\ell)| \\ &\leq C|\Lambda_0||B_n(\ell)| \leq Cn^3. \end{aligned}$$

It remains to estimate $|\mathscr{B}_n(\ell) \cap (\Lambda_0^c \times \Lambda_0^c)\,|$. There exists $C > 0$ such that for all $(\ell_1, \ell_2) \in \mathscr{B}_n(\ell)$,

$$|\ell - \ell_1| + |\ell - \ell_2| \le C|\ell_1 - \ell_2| \le Cn. \tag{6.25}$$

Using (6.25) and that $\Lambda_0^c \subset \Lambda^{\text{hom}}$, we deduce

$$\begin{aligned} |\mathscr{B}_n(\ell) \cap (\Lambda_0^c \times \Lambda_0^c)\,| &\le |\left(B_n(\ell) \cap \Lambda^{\text{hom}}\right) \times \left(B_n(\ell) \cap \Lambda^{\text{hom}}\right)| \\ &\le |B_n(\ell) \cap \Lambda^{\text{hom}}|^2 \le C|B_n(\ell)|^2 \le Cn^6. \end{aligned} \tag{6.26}$$

Collecting the estimates (6.24)–(6.26) yields the desired estimate (6.19). $\square$

The following result is an immediate consequence of Lemma 6.6.

Lemma 6.8. *For any $Y \in \mathscr{A}(\Lambda, \lambda) \cup \mathscr{A}(\Lambda^{\text{hom}}, \lambda)$ and $\gamma > 0$, there exists $C = C(\gamma, \lambda) > 0$ such that for all $\ell, n \in \text{Dom(Y)}$*

$$e^{-\gamma r_{\ell n}} \le Ce^{-\gamma|\ell - n|/2}. \tag{6.27}$$

An important consequence of Lemma 6.8 is that the locality estimates can be written as

$$|E_{\ell,n}(Y)| \le Ce^{-\gamma r_{\ell n}} \le Ce^{-\gamma|\ell-n|/2} \quad \text{for all } \ell, n \in \text{Dom(Y)}.$$

Proof of Lemma 6.8. Fix $\gamma > 0$. We show (6.8) for $Y \in \mathscr{A}(\Lambda, \lambda)$ and remark that the proof can be applied verbatim in the case $Y \in \mathscr{A}(\Lambda^{\text{hom}}, \lambda)$.

Let $\ell, n \in \Lambda$ and let $\rho = n - \ell \in \Lambda - \ell$. By Lemma 6.6 there exists a path $\mathscr{P}(\ell, \ell + \rho) = \{\ell_i \in \Lambda | 1 \le i \le N_\rho + 1\}$ of neighbouring lattice points, such that $N_\rho \le C_0|\rho|$ and $\rho_i := \ell_{i+1} - \ell_i \in \mathscr{N}(\ell_i) - \ell_i$ for all $1 \le i \le N_\rho$, satisfying

$$
\begin{aligned}
|U(\ell)-U(n)| = |D_\rho U(\ell)| &\le \sum_{i=1}^{N_\rho} |D_{\rho_i}U(\ell_i)| \le N_\rho^{1/2}\left(\sum_{i=1}^{N_\rho} |D_{\rho_i}U(\ell_i)|^2\right)^{1/2} \\
&\le C_0^{1/2}|\ell-n|^{1/2}\left(\sum_{i=1}^{N_\rho} |D_{\rho_i}U(\ell_i)|^2\right) \\
&\le C_0^{1/2}|\ell-n|^{1/2}\left(\sum_{\ell'\in\Lambda}\sum_{\rho'\in\mathscr{N}(\ell')-\ell'} |D_{\rho'}U(\ell')|^2\right)^{1/2} \\
&= C_0^{1/2}\|DU\|_{\ell^2}|\ell-n|^{1/2}. \qquad (6.28)
\end{aligned}
$$

Choosing $R := 4C_0\lambda^2$ ensures that for $|\ell - n| \ge R$

$$
|U(\ell)-U(n)| \le C_0^{1/2}\|DU\|_{\ell^2}|\ell-n|^{1/2} \le \frac{R^{1/2}|\ell-n|^{1/2}}{2} \le \frac{|\ell-n|}{2}. \qquad (6.29)
$$

Using the triangle inequality and applying (6.29), for $\ell, n \in \Lambda$ satisfying $|\ell - n| \ge R$

$$
|Y(\ell)-Y(n)| \ge |\ell-n| - |U(\ell)-U(n)| \ge \frac{|\ell-n|}{2},
$$

hence $e^{-\gamma|Y(\ell)-Y(n)|} \le e^{-\gamma|\ell-n|/2}$. When $|\ell - n| < R$, as $|Y(\ell) - Y(n)| \ge 0$

$$
e^{-\gamma|Y(\ell)-Y(n)|} \le 1 \le e^{\gamma R/2}e^{-\gamma|\ell-n|/2},
$$

so the desired estimate (6.27) holds. □

6.6.2 Equivalent norms

The exponential decay of the site energy motivates us to define a family of norms using exponentially-weighted finite-difference stencils: for $\gamma > 0$, define

$$
\big|DU(\ell)\big|_\gamma := \sum_{\rho\in\Lambda-\ell} e^{-\gamma|\rho|}\big|D_\rho U(\ell)\big| \quad \text{and} \quad \|DU\|_{\ell^2_\gamma} := \left(\sum_{\ell\in\Lambda} |DU(\ell)|_\gamma^2\right)^{1/2}. \qquad (6.30)
$$

The following lemma shows the equivalence between the norms $\|D\cdot\|_{\ell^2_\gamma}$ and $\|D\cdot\|_{\ell^2}$.

Lemma 6.9. *Let $\gamma > 0$, then there exist constants $c_\gamma, C_\gamma > 0$ such that*

$$c_\gamma \|DU\|_{\ell^2} \le \|DU\|_{\ell^2_\gamma} \le C_\gamma \|DU\|_{\ell^2} \qquad \forall\, U \in \dot{\mathscr{W}}^{1,2}. \tag{6.31}$$

Proof of Lemma 6.9. Fix $\gamma > 0$. We first show that

$$c_\gamma \|DU\|_{\ell^2} \le \|DU\|_{\ell^2_\gamma}. \tag{6.32}$$

From the assumption **(RC)** on Page 155, there exists $c_0 > 0$ such that

$$\max_{\ell\in\Lambda} \max_{\rho\in\mathcal{N}(\ell)-\ell} |\rho| = c_0 > 0,$$

hence $e^{-\gamma|\rho|} \ge e^{-\gamma c_0} > 0$ for all $\ell \in \Lambda$ and $\rho \in \mathcal{N}(\ell) - \ell$. Using the embedding $\ell^1 \subset \ell^2$

$$\begin{aligned}
\big|DU(\ell)\big|_{\mathscr{N}} = \bigg(\sum_{\rho\in\mathscr{N}(\ell)-\ell} \big|D_\rho U(\ell)\big|^2\bigg)^{1/2} &\le \sum_{\rho\in\mathscr{N}(\ell)-\ell} \big|D_\rho U(\ell)\big| \\
&\le e^{\gamma c_0} \sum_{\rho\in\mathscr{N}(\ell)-\ell} e^{-\gamma|\rho|}\big|D_\rho U(\ell)\big| \le e^{\gamma c_0}\big|DU(\ell)\big|_\gamma.
\end{aligned}$$

This implies (6.32) as

$$\|DU\|_{\ell^2} = \bigg(\sum_{\ell\in\Lambda} |DU(\ell)|^2_{\mathscr{N}}\bigg)^{1/2} \le e^{\gamma c_0}\bigg(\sum_{\ell\in\Lambda} |DU(\ell)|^2_{\mathfrak{w},k}\bigg)^{1/2} = e^{\gamma c_0}\|DU\|_{\ell^2_{\mathfrak{w},k}}.$$

We now show the remaining estimate. Applying Cauchy–Schwarz gives

$$\begin{aligned}
|DU(\ell)|_\gamma = \sum_{\rho\in\Lambda-\ell} e^{-\gamma|\rho|}\big|D_\rho U(\ell)\big| &= \sum_{\rho\in\Lambda-\ell} e^{\gamma|\rho|/2}\left(e^{-\gamma|\rho|/2}\big|D_\rho U(\ell)\big|\right) \\
&\le \bigg(\sum_{\rho\in\Lambda-\ell} e^{-\gamma|\rho|/2}\bigg)^{1/2}\bigg(\sum_{\rho\in\Lambda-\ell} e^{-\gamma|\rho|}\big|D_\rho U(\ell)\big|^2\bigg)^{1/2}.
\end{aligned} \tag{6.33}$$

By Lemma 6.6, for each $\ell \in \Lambda$ and $\rho \in \Lambda - \ell$, there exists a path $\mathscr{P}(\ell, \ell+\rho) = \{\ell_i \in \Lambda | 1 \le i \le N_\rho + 1\}$ of neighbouring lattice points, such that $N_\rho \le C|\rho|$ and $\rho_i := \ell_{i+1} - \ell_i \in \mathscr{N}(\ell_i) - \ell_i$ for all $1 \le i \le N_\rho$, satisfying

$$|D_\rho U(\ell)| \le \sum_{i=1}^{N_\rho} |D_{\rho_i} U(\ell_i)|.$$

Applying Cauchy–Schwarz again gives

$$|D_\rho U(\ell)|^2 \le \bigg(\sum_{i=1}^{N_\rho} |D_{\rho_i} U(\ell_i)|\bigg)^2 \le N_\rho \sum_{i=1}^{N_\rho} |D_{\rho_i} U(\ell_i)|^2 \le C|\rho| \sum_{i=1}^{N_\rho} |D_{\rho_i} U(\ell_i)|^2. \tag{6.34}$$

Combining (6.33)–(6.34) gives

$$\begin{aligned}
\|DU\|_{\ell^2_\gamma} = \bigg(\sum_{\ell\in\Lambda} |DU(\ell)|^2_\gamma\bigg)^{1/2} &\le C\gamma^{-3/4}\bigg(\sum_{\ell\in\Lambda}\sum_{\rho\in\Lambda-\ell} e^{-\gamma|\rho|}|D_\rho U(\ell)|^2\bigg)^{1/2} \\
&\le C\bigg(\sum_{\ell\in\Lambda}\sum_{\rho\in\Lambda-\ell} e^{-\gamma|\rho|}|\rho| \sum_{i=1}^{N_\rho} |D_{\rho_i} U(\ell_i)|^2\bigg)^{1/2} \\
&\le C\bigg(\sum_{\ell\in\Lambda}\sum_{\rho\in\Lambda-\ell} e^{-\gamma|\rho|}|\rho| \sum_{i=1}^{N_\rho} \sum_{\rho'\in\mathscr{N}(\ell_i)-\ell_i} |D_{\rho'} U(\ell_i)|^2\bigg)^{1/2} \\
&= C\bigg(\sum_{\ell'\in\Lambda}\sum_{\rho'\in\mathscr{N}(\ell')-\ell'} |D_{\rho'} U(\ell')|^2 \sum_{\ell\in\Lambda} \sum_{\substack{\rho\in\Lambda-\ell \\ \ell'\in\mathscr{P}(\ell,\ell+\rho)}} e^{-\gamma|\rho|}|\rho|\bigg)^{1/2}
\end{aligned} \tag{6.35}$$

By Lemma 6.7, for all $\ell' \in \Lambda$ and $n \in \mathbb{N}$, the set

$$\mathscr{B}_n(\ell') = \left\{(\ell_1,\ell_2)\in\Lambda^2 \,\middle|\, n-1 < |\ell_1-\ell_2| \le n, \ell' \in \mathscr{P}(\ell_1,\ell_2)\right\}$$

satisfies $|\mathscr{B}_n(\ell')| \le Cn^6$. As $e^{-\gamma|\cdot|}$ is a decreasing function, it follows that

$$\begin{aligned}
\sum_{\ell\in\Lambda} \sum_{\substack{\rho\in\Lambda-\ell \\ \ell'\in\mathscr{P}(\ell,\ell+\rho)}} e^{-\gamma|\rho|}|\rho| &= \sum_{n=1}^{\infty} \sum_{\ell_1,\ell_2\in\mathscr{B}_n(\ell')} e^{-\gamma|\ell_1-\ell_2|}|\ell_1-\ell_2| \\
&\le C\sum_{n=1}^{\infty} e^{-\gamma(n-1)} n^6 =: C_1.
\end{aligned} \tag{6.36}$$

Combining (6.35)–(6.36) we obtain the desired result

$$\|DU\|_{\ell^2_\gamma} \le C\Big(\sum_{\ell'\in\Lambda}\sum_{\rho'\in\mathscr{N}(\ell')-\ell'} |D_{\rho'}U(\ell')|^2 \sum_{\ell\in\Lambda}\sum_{\substack{\rho\in\Lambda-\ell\\ \ell'\in\mathscr{P}(\ell,\ell+\rho)}} e^{-\gamma|\rho|}|\rho|\Big)^{1/2}$$
$$\le CC_1^{1/2}\Big(\sum_{\ell'\in\Lambda}\sum_{\rho'\in\mathscr{N}(\ell')-\ell'} |D_{\rho'}U(\ell')|^2\Big)^{1/2} = C\|DU\|_{\ell^2}.$$

□

6.6.3 Interpolation between Λ and $\Lambda^{\rm hom}$

The homogeneity estimates **(SE.H)** allows us to compare site energies between defective and homogeneous configurations. In order to fully utilise these results, we require interpolation operators for displacements from Λ to $\Lambda^{\rm hom}$ and vice versa.

Lemma 6.10. *There exists a bounded linear operator* $I^{\rm hom} : \dot{\mathscr{W}}^{1,2}(\Lambda) \to \dot{\mathscr{W}}^{1,2}(\Lambda^{\rm hom})$ *satisfying:*

1. $I^{\rm hom}U(\ell) = U(\ell)$ *for* $\ell \in \Lambda^{\rm hom} \setminus B_{R_{\rm def}}$*,*
2. *there exist* $C > 0$ *such that for all* $r > 0$*, there exists* $R \ge r$ *satisfying*

$$\sum_{\ell\in\Lambda^{\rm hom}\cap B_r} |DI^{\rm hom}U(\ell)|_\gamma \le C \sum_{\ell\in\Lambda\cap B_R} |DU(\ell)|_\gamma \quad \text{for all } U \in \dot{\mathscr{W}}^{1,2}(\Lambda). \tag{6.37}$$

Moreover, for all $\gamma > 0$

$$\|DI^{\rm hom}U\|_{\ell^2_\gamma(\Lambda^{\rm hom})} \le C\|DU\|_{\ell^2_\gamma(\Lambda)} \quad \text{for all } U \in \dot{\mathscr{W}}^{1,2}(\Lambda). \tag{6.38}$$

Lemma 6.11. *There exists a bounded linear operator* $I^{\rm def} : \dot{\mathscr{W}}^{1,2}(\Lambda^{\rm hom}) \to \dot{\mathscr{W}}^{1,2}(\Lambda)$ *satisfying:*

1. $I^{\rm def}U^{\rm hom}(\ell) = U^{\rm hom}(\ell)$ *for* $\ell \in \Lambda \setminus B_{R_{\rm def}}$*,*

2. there exist $r, R, C > 0$ such that for all $U^{\mathrm{hom}} \in \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})$ and $\gamma > 0$

$$\sum_{\ell \in \Lambda \cap B_r} |DI^{\mathrm{def}}U^{\mathrm{hom}}(\ell)|_\gamma \leq C \sum_{\ell \in \Lambda^{\mathrm{hom}} \cap B_R} |DU^{\mathrm{hom}}(\ell)|_\gamma, \tag{6.39}$$
$$\|DI^{\mathrm{def}}U^{\mathrm{hom}}\|_{\ell^2_\gamma(\Lambda)} \leq C\|DU^{\mathrm{hom}}\|_{\ell^2_\gamma(\Lambda^{\mathrm{hom}})}.$$

Remark 24. For fixed $\lambda > 0$, define

$$\lambda' = \lambda \cdot \max\left\{\|I^{\mathrm{hom}}\|_{\dot{\mathscr{W}}^{1,2}(\Lambda),\dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})}, \|I^{\mathrm{def}}\|_{\dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}}),\dot{\mathscr{W}}^{1,2}(\Lambda)}\right\} > 0. \tag{6.40}$$

It follows that $I^{\mathrm{hom}} : \dot{\mathscr{W}}^{1,2}(\Lambda, \lambda) \to \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}}, \lambda')$ and $I^{\mathrm{def}} : \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}}, \lambda) \to \dot{\mathscr{W}}^{1,2}(\Lambda, \lambda')$. Consequently, the site energy estimates **(SE.L)**, **(SE.H)** will continue to be uniform for the interpolated displacements, though the constants appearing in these estimates will now depend on λ' instead of λ. □

Proof of Lemma 6.10. Fix $\gamma > 0$, $U \in \dot{\mathscr{W}}^{1,2}(\Lambda)$ and for $\ell \in \Lambda^{\mathrm{hom}} \setminus B_{R_{\mathrm{def}}}$ define $I^{\mathrm{hom}}U(\ell) = U(\ell)$. Due to the periodicity of Λ^{hom}, for each $\ell \in \Lambda^{\mathrm{hom}}$ there exists a bounded Voronoi cell $\mathcal{V}^{\mathrm{hom}}(\ell) \subset B_{\widetilde{R}}(\ell)$, where $\widetilde{R} = \frac{1}{2}\sum_{i=1}^{3}|Ae_i| > 0$, satisfying

$$\mathcal{V}^{\mathrm{hom}}(\ell) = \left\{ x \in \mathbb{R}^3 \,\middle|\, |x-\ell| \leq |x-k| \quad \forall\, k \in \Lambda^{\mathrm{hom}} \right\}$$

and $\mathcal{V}^{\mathrm{hom}}(\ell) = \mathcal{V}^{\mathrm{hom}}(0) + \ell$, due to the translation-invariance of Λ^{hom}. Using the definition (6.20), one may also define the Voronoi cell $\mathcal{V}(\ell)$ for $\ell \in \Lambda$. As $\Lambda \setminus B_{R_{\mathrm{def}}} = \Lambda^{\mathrm{hom}} \setminus B_{R_{\mathrm{def}}}$, there exists $R' > 0$ such that $\ell \in \Lambda \setminus B_{R'}$ guarantees $\mathcal{V}(\ell) = \mathcal{V}^{\mathrm{hom}}(\ell) \subset B_{\widetilde{R}}(\ell)$, which is bounded. As $\{\mathcal{V}(\ell) | \ell \in \Lambda\}$ cover $\mathbb{R}^3$, it follows from the definition (6.20) that for $\ell \in \Lambda \cap B_{R'}$

$$\mathcal{V}(\ell) \subset \bigcup_{\ell' \in \Lambda \cap B_{R'}} \mathcal{V}(\ell') \subset \left(\left(\bigcup_{\ell' \in \Lambda \setminus B_{R'}} \mathcal{V}(\ell')\right)^{\mathrm{o}}\right)^{\mathrm{c}}, \tag{6.41}$$

where X^{o} denotes the interior of the set X. As the right-hand side of (6.41) is a bounded set, there exists $R_0 > 0$ such that $\mathcal{V}(\ell) \subset B_{R_0}(\ell)$ for all $\ell \in \Lambda$.

In addition, there exists $R_1 > 0$ such that

$$\Lambda^{\rm hom} \cap B_{R_{\rm def}} \subset \bigcup_{\ell' \in \Lambda \cap B_{R_1}} \mathcal{V}(\ell'),$$

hence for each $\ell \in \Lambda^{\rm hom} \cap B_{R_{\rm def}}$, there exists $\ell' \in \Lambda \cap B_{R_1}$ such that $\ell \in \mathcal{V}(\ell') \subset B_{R_0}(\ell')$. Note that the choice of ℓ' is in general not unique. Then define $I^{\rm hom}U(\ell) = U(\ell')$. It follows from the construction that $I^{\rm hom}$ is linear.

We now show the estimates (6.37)–(6.38). Consider $\ell_1, \ell_2 \in \Lambda^{\rm hom} \cap B_{R_{\rm def}}$, then for $i = 1, 2$ there exist $\ell_i' \in \Lambda \cap B_{R_1}$ such that $I^{\rm hom}U(\ell_i) = U(\ell_i')$ and $|\ell_i - \ell_i'| \leq R_0$, hence the triangle inequality implies

$$\begin{aligned} e^{-\gamma|\ell_1-\ell_2|}|I^{\rm hom}U(\ell_1) - I^{\rm hom}U(\ell_2)| &= e^{-\gamma|\ell_1-\ell_2|}|U(\ell_1') - U(\ell_2')| \\ \leq e^{2\gamma R_0} e^{-\gamma|\ell_1'-\ell_2'|}|U(\ell_1') - U(\ell_2')| &\leq C \sum_{\ell' \in \Lambda \cap B_{R_1}} e^{-\gamma|\ell_1'-\ell'|}|U(\ell_1') - U(\ell')|. \end{aligned} \tag{6.42}$$

In the case $\ell_1 \in \Lambda^{\rm hom} \cap B_{R_{\rm def}}$ and $\ell_2 \in \Lambda^{\rm hom} \setminus B_{R_{\rm def}}$, then $I^{\rm hom}U(\ell_2) = U(\ell_2)$, then a similar argument shows

$$e^{-\gamma|\ell_1-\ell_2|}|I^{\rm hom}U(\ell_1) - I^{\rm hom}U(\ell_2)| \leq e^{\gamma R_0} e^{-\gamma|\ell_1'-\ell_2|}|U(\ell_1') - U(\ell_2)|. \tag{6.43}$$

Now, we decompose

$$\begin{aligned} |DI^{\rm hom}U(\ell_1)|_\gamma &= \sum_{\rho \in \Lambda_*^{\rm hom}} e^{-\gamma|\rho|}|D_\rho I^{\rm hom}U(\ell_1)| \\ &= \sum_{\ell_2 \in \Lambda^{\rm hom}} e^{-\gamma|\ell_1-\ell_2|}|I^{\rm hom}U(\ell_1) - I^{\rm hom}U(\ell_2)| \\ &= \sum_{\ell_2 \in \Lambda^{\rm hom} \cap B_{R_{\rm def}}} e^{-\gamma|\ell_1-\ell_2|}|I^{\rm hom}U(\ell_1) - I^{\rm hom}U(\ell_2)| \\ &\qquad + \sum_{\ell_2 \in \Lambda^{\rm hom} \setminus B_{R_{\rm def}}} e^{-\gamma|\ell_1-\ell_2|}|I^{\rm hom}U(\ell_1) - I^{\rm hom}U(\ell_2)|, \end{aligned}$$

then combine (6.42)–(6.43) to deduce

$$
\begin{aligned}
|DI^{\mathrm{hom}}U(\ell_1)|_\gamma &\le C|\Lambda^{\mathrm{hom}} \cap B_{R_{\mathrm{def}}}| \sum_{\ell' \in \Lambda \cap B_{R_1}} e^{-\gamma|\ell_1' - \ell'|}|U(\ell_1') - U(\ell')| \\
&\quad + C \sum_{\ell' \in \Lambda \setminus B_{R_{\mathrm{def}}}} e^{-\gamma|\ell_1' - \ell'|}|U(\ell_1') - U(\ell_2')| \\
&\le C \sum_{\ell_2' \in \Lambda \setminus \ell_1'} e^{-\gamma|\ell_1' - \ell_2'|}|U(\ell_1') - U(\ell_2')| = C \sum_{\rho' \in \Lambda - \ell_1'} e^{-\gamma|\rho'|}|D_{\rho'}U(\ell_1')| \\
&= C|DU(\ell_1')|_\gamma \le C \sum_{\ell' \in \Lambda \cap B_{R_1}} |DU(\ell')|_\gamma. \qquad (6.44)
\end{aligned}
$$

An identical argument shows that for $\ell_1 \in \Lambda^{\mathrm{hom}} \cap B_{R_{\mathrm{def}}}$, as $\ell_1 = \ell_1'$

$$
|DI^{\mathrm{hom}}U(\ell_1)|_\gamma \le C|DU(\ell_1)|_\gamma. \qquad (6.45)
$$

Let $r > 0$ and choose $R = \max\{R_1, r\}$, then combining (6.44)–(6.45) yields (6.37)

$$
\sum_{\ell \in \Lambda^{\mathrm{hom}} \cap B_r} |DI^{\mathrm{hom}}U(\ell)|_\gamma \le C \sum_{\ell \in \Lambda \cap B_R} |DU(\ell)|_\gamma.
$$

We now show (6.38) using (6.44)–(6.45) and Cauchy–Schwarz

$$
\begin{aligned}
\|DI^{\mathrm{hom}}U\|^2_{\ell^2_\gamma(\Lambda^{\mathrm{hom}})} &= \sum_{\ell \in \Lambda^{\mathrm{hom}}} |DI^{\mathrm{hom}}U(\ell)|^2_\gamma \\
&= \sum_{\ell \in \Lambda^{\mathrm{hom}} \cap B_{R_{\mathrm{def}}}} |DI^{\mathrm{hom}}U(\ell)|^2_\gamma + \sum_{\ell \in \Lambda^{\mathrm{hom}} \setminus B_{R_{\mathrm{def}}}} |DI^{\mathrm{hom}}U(\ell)|^2_\gamma \\
&\le C \sum_{\ell \in \Lambda^{\mathrm{hom}} \cap B_{R_{\mathrm{def}}}} \Bigg(\sum_{\ell' \in \Lambda \cap B_{R_1}} |DU(\ell')|_\gamma \Bigg)^2 + C \sum_{\ell \in \Lambda \setminus B_{R_{\mathrm{def}}}} |DU(\ell)|^2_\gamma \\
&\le C|B_{R_1}| \sum_{\ell \in \Lambda^{\mathrm{hom}} \cap B_{R_{\mathrm{def}}}} \sum_{\ell' \in \Lambda \cap B_{R_1}} |DU(\ell')|^2_\gamma + C \sum_{\ell \in \Lambda \setminus B_{R_{\mathrm{def}}}} |DU(\ell)|^2_\gamma \\
&\le C|\Lambda^{\mathrm{hom}} \cap B_{R_{\mathrm{def}}}| \sum_{\ell' \in \Lambda \cap B_{R_1}} |DU(\ell')|^2_\gamma + C \sum_{\ell' \in \Lambda \setminus B_{R_{\mathrm{def}}}} |DU(\ell')|^2_\gamma \\
&\le C \sum_{\ell' \in \Lambda} |DU(\ell')|^2_\gamma = C\|DU\|^2_{\ell^2_\gamma(\Lambda)}.
\end{aligned}
$$

□

Proof of Lemma 6.11. This holds from following the proof of Lemma 6.10 verbatim. $\square$

6.7 Proof of site energy results

We now prove the results discussed in Section 6.2.

Proof of Lemma 6.2. We prove that each $Y \in \mathscr{A}(\Lambda, \lambda)$ defines $m_Y \in \mathcal{M}_{L^2}(M, \omega)$ and remark that our proof also holds for $Y^{\mathrm{hom}} \in \mathscr{A}(\Lambda^{\mathrm{hom}})$.

In the following argument, we apply the Gagliardo–Nirenberg–Sobolev (GNS) estimate for discrete functions: for all $U \in \dot{\mathscr{W}}^{1,2}(\Lambda)$, there exist $U_0 \in \ell^6(\Lambda) \cap \dot{\mathscr{W}}^{1,2}(\Lambda)$, $c \in \mathbb{R}^3$ such that $U = U_0 + c$ and as $\ell^6(\Lambda) \hookrightarrow \ell^\infty(\Lambda)$

$$\|U_0\|_{\ell^\infty(\Lambda)} \leq \|U_0\|_{\ell^6(\Lambda)} \leq C_* \|DU_0\|_{\ell^2(\Lambda)} = C_* \|DU\|_{\ell^2(\Lambda)}, \tag{6.46}$$

where the constant C_* is independent of U. This follows from [54, Proposition 12] and [55]. Let $Y = Y_0 + U = Y_0 + U_0 + c$ denote the deformation corresponding to U and recall (6.3), which defines the nuclear density

$$m(x) = m_Y(x) = \sum_{\ell \in \Lambda} \eta(x - Y(\ell)) = \sum_{\ell \in \Lambda} \eta(x - c - \ell - U_0(\ell)),$$

where $\int_{\mathbb{R}^3} \eta = 1$, $\mathrm{spt}(\eta) \subset B_{R_0}(0)$ and we have used the GNS embedding to obtain the final term.

Due to the periodic arrangement of Λ^{hom}, there exist $C_0', C_1', C_2' > 0$ such that for all $r > 0$ and $x \in \mathbb{R}^3$

$$C_0' r^3 - C_1' \leq \left|\Lambda^{\mathrm{hom}} \cap B_r(x)\right| \leq C_2' r^3.$$

Moreover, as the assumption **(RC)** ensures that $|\Lambda \cap B_{R_{\mathrm{def}}}(0)| < \infty$ and $\Lambda \setminus B_{R_{\mathrm{def}}}(0) = \Lambda^{\mathrm{hom}} \setminus B_{R_{\mathrm{def}}}(0)$, there exists $C_0, C_1, C_2, C_3 > 0$ such that for all $r > 0$ and $x \in \mathbb{R}^3$

$$C_0 r^3 - C_1 \leq |\Lambda \cap B_r(x)| \leq C_2 r^3 + C_3. \tag{6.47}$$

For $x \in \mathbb{R}^3$, applying (6.46)–(6.47), we obtain

$$\int_{B_1(x)} m \le \left|B_{1+R_0+\|U_0\|_{\ell^\infty(\Lambda)}}(x-c)\right| \int_{\mathbb{R}^3} \eta \le C_2 \left(1 + R_0 + \|U_0\|_{\ell^\infty(\Lambda)}\right)^3 + C_3$$
$$\le C(1 + \|DU\|^3_{\ell^2(\Lambda)}) \le C(1+\lambda^3) =: M.$$

Similarly, for $R \ge R_1 := 2\,(R_0 + C_*\lambda)$, by applying (6.46) we deduce

$$\begin{aligned}\int_{B_R(x)} m &\ge \left|B_{R-R_0-\|U_0\|_{\ell^\infty(\Lambda)}}(x-c)\right| \int_{\mathbb{R}^3} \eta \\ &\ge C_0 \left(R - R_0 - \|U\|_{\ell^\infty(\Lambda)}\right)^3 - C_1 \\ &\ge C_0 \left(R - R_0 - C_*\|DU\|_{\ell^2(\Lambda)}\right)^3 - C_1 \\ &\ge C_0 \left(R - R_0 - C_*\lambda\right)^3 - C_1 \ge \frac{C_0}{8} R^3 - C_1.\end{aligned}$$

hence $m_Y \in \mathcal{M}_{L^2}(M, \omega)$, for $\omega = (\omega_0, \omega_1) = (\frac{C_0}{8}, C_1 + \frac{C_0}{8} R_1^3)$.

$\square$

We now prove Proposition 6.3. Other than the homogeneity estimates **(SE.H)**, the results of Proposition 6.3 follow directly from the estimates established in Chapter 5. We now state **(SE.H)** as a separate lemma.

Lemma 6.12. *Let $Y_1, Y_2 \in \mathscr{A}(\Lambda, \lambda) \cup \mathscr{A}(\Lambda^{\mathrm{hom}}, \lambda)$ and for $i = 1, 2$, let $\Lambda_i' = \mathrm{Dom}(Y_i)$. There exist $C = C(\lambda), \gamma = \gamma(\lambda) > 0$ such that for any $\ell_1 \in \Lambda_1', \ell_2 \in \Lambda_2'$ and $r \ge 0$ satisfying*

$$\begin{aligned}&\{Y_1(n_1) - Y_1(\ell_1) \mid n_1 \in \Lambda_1' \text{ s.t. } r_{\ell_1 n_1}(Y_1) \le r\} \\ &= \{Y_2(n_2) - Y_2(\ell_2) \mid n_2 \in \Lambda_2' \text{ s.t. } r_{\ell_2 n_2}(Y_2) \le r\},\end{aligned} \tag{6.48}$$

then

$$|E_{\ell_1}(Y_1) - E_{\ell_2}(Y_2)| \le C e^{-\gamma r}, \tag{6.49}$$

Additionally, for any $n_1 \in \Lambda_1' \setminus \ell_1$ satisfying $r_{\ell_1 n_1}(Y_1) \le r$ there exists unique $n_2 \in \Lambda_2' \setminus \ell_2$ satisfying $Y_1(n_1) - Y_1(\ell_1) = Y_2(n_2) - Y_2(\ell_2)$ and

$$|E_{\ell_1,n_1}(Y_1) - E_{\ell_2,n_2}(Y_2)| \le C e^{-\gamma(r + r_{\ell_1 n_1})}. \tag{6.50}$$

Due to the length of the argument, we postpone the proof of Lemma 6.12. Instead, we now prove Proposition 6.3 under the assumption that Lemma 6.12 holds.

Proof of Proposition 6.3. The symmetry properties **(SE.P)** and **(SE.I)** follows directly from Remark 12 in Chapter 5.

We now show **(SE.R)** and **(SE.L)**, so let $Y \in \mathscr{A}(\Lambda, \lambda)$ and $U \in \dot{\mathscr{W}}^{1,2}(\Lambda)$. There exists $t_0 > 0$ such that $Y + tU \in \mathscr{A}(\Lambda, \lambda)$ for all $0 \leq t \leq t_0$, hence by Lemma 6.2, there exist (M, ω) such that $Y + tU \in \mathcal{Y}_{L^2}(M, \omega)$ for all $0 \leq t \leq t_0$. For $\ell \in \Lambda$, $j \in \mathbb{N}$ and $\mathbf{n} = (n_1, \dots, n_j) \in \Lambda^j$, recall the definition of the partial derivative

$$E_{\ell,\mathbf{n}}(Y) = \frac{\partial^j E_\ell(Y)}{\partial Y(n_1) \cdots \partial Y(n_j)}.$$

Both regularity and locality follow from Theorem 5.11, in particular the estimate (5.85) implies

$$|E_{\ell,\mathbf{n}}(Y)| \leq C_j e^{-\gamma \sum_{i=1}^{j} r_{\ell n_i}}.$$

The homogeneity estimate **(SE.H)** then follows directly from Lemma 6.12. □

In order to prove Lemma 6.12, we first show a result comparing partition functions when (6.48) holds.

Lemma 6.13. *Let $Y_1, Y_2 \in \mathscr{A}(\Lambda, \lambda) \cup \mathscr{A}(\Lambda^{\mathrm{hom}}, \lambda)$ and for $i = 1, 2$, let $\Lambda_i' = \mathrm{Dom}(Y_i)$. Suppose Y_1, Y_2 satisfy (6.48), for some $\ell_1 \in \Lambda_1', \ell_2 \in \Lambda_2'$ and $r \geq 0$, then there exist constants $C = C(\lambda), \gamma = \gamma(\lambda) > 0$, independent of ℓ_1, ℓ_2 and r, such that*

$$|\varphi_{\ell_1}(Y_1; x + Y_1(\ell_1)) - \varphi_{\ell_2}(Y_2; x + Y_2(\ell_2))| \leq C e^{-\gamma(2|x| + r)}. \tag{6.51}$$

Additionally, for any $n_1 \in \Lambda_1' \setminus \ell_1$ satisfying $r_{\ell_1 n_1}(Y_1) \leq r$, we have

$$\left| \frac{\partial \varphi_{\ell_1}(Y_1; x + Y_1(\ell_1))}{\partial Y_1(n_1)} - \frac{\partial \varphi_{\ell_2}(Y_2; x + Y_2(\ell_2))}{\partial Y_2(n_2)} \right| \leq C e^{-\gamma(|x| + r + r_{\ell_1 n_1})}. \tag{6.52}$$

where n_2 is the unique element of $\Lambda_2' \setminus \ell_2$ satisfying $Y_1(n_1) - Y_1(\ell_1) = Y_2(n_2) - Y_2(\ell_2)$.

Proof of Lemma 6.13. By the definition (6.5)

$$\varphi_{\ell_1}(Y_1; x + Y_1(\ell_1)) = \frac{\widetilde{\varphi}(x)}{\sum_{k_1 \in \Lambda_1'} \widetilde{\varphi}(x + Y_1(\ell_1) - Y_1(k_1))},$$
$$\varphi_{\ell_2}(Y_2; x + Y_2(\ell_2)) = \frac{\widetilde{\varphi}(x)}{\sum_{k_2 \in \Lambda_2'} \widetilde{\varphi}(x + Y_2(\ell_2) - Y_2(k_2))},$$

hence

$$|\varphi_{\ell_1}(Y_1; x + Y_1(\ell_1)) - \varphi_{\ell_2}(Y_2; x + Y_2(\ell_2))|$$
$$= \widetilde{\varphi}(x) \left| \left(\sum_{k_1 \in \Lambda_1'} \widetilde{\varphi}(x + Y_1(\ell_1) - Y_1(k_1)) \right)^{-1} - \left(\sum_{k_2 \in \Lambda_2'} \widetilde{\varphi}(x + Y_2(\ell_2) - Y_2(k_2)) \right)^{-1} \right| \tag{6.53}$$

We estimate (6.53) by first considering the general expression

$$\widetilde{\varphi}(x) \left| \left(\sum_{k_1 \in \Lambda_1'} \widetilde{\varphi}(x + Y_1(\ell_1) - Y_1(k_1)) \right)^{-\alpha} - \left(\sum_{k_2 \in \Lambda_2'} \widetilde{\varphi}(x + Y_2(\ell_2) - Y_2(k_2)) \right)^{-\alpha} \right|, \tag{6.54}$$

for $\alpha \geq 1$. As $\widetilde{\varphi}(x) = e^{-\gamma|x|^2}$, the property $\bigcup_{j \in \mathbb{N}} B_{R'}(Y_j) = \mathbb{R}^3$ (5.2) ensures that

$$c_0 := \min_{i=1,2} \inf_{x \in \mathbb{R}^3} \sum_{k_i \in \Lambda_i'} \widetilde{\varphi}(x + Y_i(\ell_i) - Y_i(k_i)) > 0,$$

hence applying the Mean Value Theorem to (6.54) gives

$$\widetilde{\varphi}(x) \left| \left(\sum_{k_1 \in \Lambda_1'} \widetilde{\varphi}(x + Y_1(\ell_1) - Y_1(k_1)) \right)^{-\alpha} - \left(\sum_{k_2 \in \Lambda_2'} \widetilde{\varphi}(x + Y_2(\ell_2) - Y_2(k_2)) \right)^{-\alpha} \right|$$
$$\leq \alpha c_0^{-\alpha-1} \widetilde{\varphi}(x) \left| \sum_{k_1 \in \Lambda_1'} \widetilde{\varphi}(x + Y_1(\ell_1) - Y_1(k_1)) - \sum_{k_2 \in \Lambda_2'} \widetilde{\varphi}(x + Y_2(\ell_2) - Y_2(k_2)) \right| \tag{6.55}$$

The condition (6.48) implies

$$\sum_{\substack{k_1 \in \Lambda_1' \text{ s.t.} \\ |r_{\ell_1 k_1}| \le r}} \widetilde{\varphi}(x + Y_1(\ell_1) - Y_1(k_1)) \;=\; \sum_{\substack{k_2 \in \Lambda_2' \text{ s.t.} \\ |r_{\ell_2 k_2}| \le r}} \widetilde{\varphi}(x + Y_2(\ell_2) - Y_2(k_2)). \tag{6.56}$$

In order to estimate the remaining terms in (6.55), we first estimate

$$\begin{aligned}
&\sum_{\substack{k_1 \in \Lambda_1' \text{ s.t.} \\ |r_{\ell_1 k_1}| > r}} \widetilde{\varphi}(x + Y_1(\ell_1) - Y_1(k_1)) \\
&\quad \le \sum_{\substack{k_1 \in \Lambda_1' \text{ s.t.} \\ |r_{\ell_1 k_1}| > r}} e^{-\widetilde{\gamma}|x + Y_1(\ell_1) - Y_1(k_1)|} \le \sum_{\substack{k_1 \in \Lambda_1' \text{ s.t.} \\ |r_{\ell_1 k_1}| > r}} e^{-\widetilde{\gamma}|x + Y_1(\ell_1) - Y_1(k_1)|/2} \\
&\quad \le \sum_{\substack{k_1 \in \Lambda_1' \text{ s.t.} \\ |r_{\ell_1 k_1}| > r}} e^{\widetilde{\gamma}|x|/2} e^{-\widetilde{\gamma}|Y_1(\ell_1) - Y_1(k_1)|/2} \le e^{\widetilde{\gamma}(2|x| - r)/4} \sum_{k_1 \in \Lambda_1'} e^{-\widetilde{\gamma}|Y_1(\ell_1) - Y_1(k_1)|/4} \\
&\quad \le C e^{\widetilde{\gamma}(2|x| - r)/4}.
\end{aligned} \tag{6.57}$$

Combining (6.56)–(6.57), we deduce

$$\begin{aligned}
&\left| \sum_{k_1 \in \Lambda_1'} \widetilde{\varphi}(x + Y_1(\ell_1) - Y_1(k_1)) - \sum_{k_2 \in \Lambda_2'} \widetilde{\varphi}(x + Y_2(\ell_2) - Y_2(k_2)) \right| \\
&\quad \le \sum_{\substack{k_1 \in \Lambda_1' \text{ s.t.} \\ |r_{\ell_1 k_1}| > r}} \widetilde{\varphi}(x + Y_1(\ell_1) - Y_1(k_1)) \;+\; \sum_{\substack{k_2 \in \Lambda_2' \text{ s.t.} \\ |r_{\ell_2 k_2}| > r}} \widetilde{\varphi}(x + Y_2(\ell_2) - Y_2(k_2)) \\
&\quad \le C e^{\widetilde{\gamma}(2|x| - r)/4}.
\end{aligned} \tag{6.58}$$

Inserting (6.58) into (6.55) yields

$$\begin{aligned}
&\widetilde{\varphi}(x) \left| \left(\sum_{k_1 \in \Lambda_1'} \widetilde{\varphi}(x + Y_1(\ell_1) - Y_1(k_1)) \right)^{-\alpha} - \left(\sum_{k_2 \in \Lambda_2'} \widetilde{\varphi}(x + Y_2(\ell_2) - Y_2(k_2)) \right)^{-\alpha} \right| \\
&\le C e^{-\widetilde{\gamma}|x|} e^{\widetilde{\gamma}(2|x| - r)/4} = C e^{-\widetilde{\gamma}(2|x| + r)/4}.
\end{aligned} \tag{6.59}$$

In particular, the desired estimate (6.51) follows from (6.59), choosing $\alpha = 1$ and $\gamma = \widetilde{\gamma}/4 > 0$.

We now show (6.51), so suppose $n_1 \in \Lambda_1' \setminus \ell_1$ satisfies $r_{\ell_1 n_1}(Y_1) \le r$, then there exists unique $n_2 \in \Lambda_2' \setminus \ell_2$ satisfying $Y_1(n_1) - Y_1(\ell_1) = Y_2(n_2) - Y_2(\ell_2)$. For $i = 1, 2$, the derivative of the partition function is given by

$$\begin{aligned}
&\frac{\partial \varphi_{\ell_i}(Y_i; x + Y_i(\ell_i))}{\partial Y_i(n_i)} \\
&\qquad = \nabla \widetilde{\varphi}(x + Y_i(\ell_i) - Y_i(n_i))\, \widetilde{\varphi}(x) \Big(\sum_{k_i \in \Lambda_i'} \widetilde{\varphi}(x + Y_i(\ell_i) - Y_i(k_i)) \Big)^{-2} \\
&\qquad = \nabla \widetilde{\varphi}(x + Y_1(\ell_1) - Y_1(n_1))\, \widetilde{\varphi}(x) \Big(\sum_{k_i \in \Lambda_i'} \widetilde{\varphi}(x + Y_i(\ell_i) - Y_i(k_i)) \Big)^{-2},
\end{aligned}$$

where we have used $Y_1(n_1) - Y_1(\ell_1) = Y_2(n_2) - Y_2(\ell_2)$. It follows that

$$\begin{aligned}
&\frac{\partial \varphi_{\ell_1}(Y_1; x + Y_1(\ell_1))}{\partial Y_1(n_1)} - \frac{\partial \varphi_{\ell_2}(Y_2; x + Y_2(\ell_2))}{\partial Y_2(n_2)} \\
&= \nabla \widetilde{\varphi}(x + Y_1(\ell_1) - Y_1(n_1))\, \widetilde{\varphi}(x) \\
&\quad \cdot \left(\Big(\sum_{k_1 \in \Lambda_1'} \widetilde{\varphi}(x + Y_1(\ell_1) - Y_1(k_1)) \Big)^{-2} - \Big(\sum_{k_2 \in \Lambda_2'} \widetilde{\varphi}(x + Y_2(\ell_2) - Y_2(k_2)) \Big)^{-2} \right).
\end{aligned} \tag{6.60}$$

Applying (6.4) and (6.59) with $\alpha = 2$ to (6.60) yields the desired estimate (6.52)

$$\begin{aligned}
&\left| \frac{\partial \varphi_{\ell_1}(Y_1; x + Y_1(\ell_1))}{\partial Y_1(n_1)} - \frac{\partial \varphi_{\ell_2}(Y_2; x + Y_2(\ell_2))}{\partial Y_2(n_2)} \right| \\
&\qquad \le C e^{-\widetilde{\gamma}|x + Y_1(\ell_1) - Y_1(n_1)|} e^{-\widetilde{\gamma}(2|x| + r)/4} = C e^{-\widetilde{\gamma}(r + 2|x| + 4|x + Y_1(\ell_1) - Y_1(n_1)|)/4} \\
&\qquad \le C e^{-\widetilde{\gamma}(r + 2|x| + |x + Y_1(\ell_1) - Y_1(n_1)|)/4} \le C e^{-\widetilde{\gamma}(|x| + r + r_{\ell_1 n_1})/4},
\end{aligned}$$

where we have applied the triangle inequality to obtain the final estimate. □

Proof of Lemma 6.12. Throughout this proof, we consider $i \in \{1, 2\}$. Suppose $Y_i \in \mathscr{A}(\Lambda_i')$ satisfy (6.48) for $r \ge 0$, then define

$$m_i(x) = m_{Y_i}(x + Y_i(\ell_i)) = \sum_{\ell \in \Lambda_i'} \eta(x + Y_i(\ell_i) - Y_i(\ell)),$$

and let (u_i, ϕ_i) denote the corresponding ground state.

First suppose (6.48) holds for $r \leq 4R_0$, where $\mathrm{spt}(\eta) \subset B_{R_0}(0)$. Then (6.49) holds trivially as

$$|E_{\ell_1}(Y_1) - E_{\ell_2}(Y_2)| \leq |E_{\ell_1}(Y_1)| + |E_{\ell_2}(Y_2)| \leq Cc_0^{-1} \int_{\mathbb{R}^3} \widetilde{\varphi} \leq C \leq Ce^{\gamma R_0} e^{-\gamma r/4}.$$

Similarly, we show (6.50) by applying **(SE.L)** from Proposition 6.3 and using that $r_{\ell_1 n_1} = r_{\ell_2 n_2}$

$$\begin{aligned}|E_{\ell_1,n_1}(Y_1) - E_{\ell_2,n_2}(Y_2)| &\leq |E_{\ell_1,n_1}(Y_1)| + |E_{\ell_2,n_2}(Y_2)| \leq Ce^{-\gamma r_{\ell_1 n_1}} \\ &\leq Ce^{4\gamma R_0} e^{-\gamma(r + r_{\ell_1 n_1})}.\end{aligned}$$

Now consider the case that (6.48) holds for $r \geq 4R_0$, where $\mathrm{spt}(\eta) \subset B_{R_0}(0)$. Then the assumption (6.48) implies that $m_1 = m_2$ on B_{r-R_0}. As $r \geq r_0 = 4R_0$, applying Proposition 4.1, there exists $C, \gamma' > 0$ such that for all $|x| \leq r/2$

$$\sum_{|\alpha| \leq 2} |\partial^\alpha (u_1 - u_2)(x)| + |(\phi_1 - \phi_2)(x)| \leq Ce^{-\gamma'(r - R_0 - |x|)} \leq Ce^{-\gamma' r/4}. \tag{6.61}$$

As the partition function satisfies (5.6b), $\varphi_{\ell_i}(Y_i; x + Y_i(\ell_i)) \leq Ce^{-\widetilde{\gamma}|x|}$. Now recall the definition of the energy density (5.92), then define

$$\mathcal{E}_{1,i} = |\nabla u_i|^2 + u_i^{10/3} + \frac{1}{2}\phi_i(m_i - u_i^2).$$

The site energies (6.6), can be expressed as

$$E_{\ell_i}(Y_i) = \int_{\mathbb{R}^3} \mathcal{E}_{1,i}(x)\, \varphi_{\ell_i}(Y_i; x + Y_i(\ell_i))\, \mathrm{d}x,$$

hence the difference becomes

$$
\begin{aligned}
&E_{\ell_1}(Y_1) - E_{\ell_2}(Y_2) \\
&\quad = \int_{\mathbb{R}^3} \mathcal{E}_{1,1}(x)\, \varphi_{\ell_1}(Y_1; x + Y_1(\ell_1))\ \mathrm{d}x - \int_{\mathbb{R}^3} \mathcal{E}_{1,2}(x)\, \varphi_{\ell_2}(Y_2; x + Y_2(\ell_2))\ \mathrm{d}x \\
&\quad = \int_{\mathbb{R}^3} \Big(\mathcal{E}_{1,1}(x) - \mathcal{E}_{1,2}(x)\Big) \varphi_{\ell_1}(Y_1; x + Y_1(\ell_1))\ \mathrm{d}x \qquad (6.62) \\
&\qquad + \int_{\mathbb{R}^3} \mathcal{E}_{1,2}(x) \Big(\varphi_{\ell_1}(Y_1; x + Y_1(\ell_1)) - \varphi_{\ell_2}(Y_2; x + Y_2(\ell_2))\Big)\ \mathrm{d}x. \qquad (6.63)
\end{aligned}
$$

We decompose the integral (6.62) into

$$
\begin{aligned}
&\int_{B_{r/2}(0)} \Big(\mathcal{E}_{1,1}(x) - \mathcal{E}_{1,2}(x)\Big) \varphi_{\ell_1}(Y_1; x + Y_1(\ell_1))\ \mathrm{d}x \qquad (6.64) \\
&\qquad + \int_{B_{r/2}(0)^{\mathrm{c}}} \Big(\mathcal{E}_{1,1}(x) - \mathcal{E}_{1,2}(x)\Big) \varphi_{\ell_1}(Y_1; x + Y_1(\ell_1))\ \mathrm{d}x. \qquad (6.65)
\end{aligned}
$$

We estimate (6.64) using that $m_1 = m_2$ on $B_{r/2}(0)$, applying (6.61) and Proposition 2.1, we deduce for $|x| \le r/2$

$$
\begin{aligned}
|(\mathcal{E}_{1,1} - \mathcal{E}_{1,2})(x)| &\le C\left(|\nabla(u_1 - u_2)(x)| + |(u_1 - u_2)(x)| + |(\phi_1 - \phi_2)(x)|\right) \\
&\le C e^{-\gamma' r/4},
\end{aligned}
$$

hence

$$
\begin{aligned}
&\left| \int_{B_{r/2}(0)} \Big(\mathcal{E}_{1,1}(x) - \mathcal{E}_{1,2}(x)\Big) \varphi_{\ell_1}(Y_1; x + Y_1(\ell_1))\ \mathrm{d}x \right| \\
&\qquad \le C e^{-\gamma' r/4} \int_{B_{r/2}(0)} \varphi_{\ell_1}(Y_1; x + Y_1(\ell_1))\ \mathrm{d}x \le C e^{-\gamma' r/4}.
\end{aligned}
$$

Then, (6.65) is estimated by

$$
\begin{aligned}
&\left| \int_{B_{r/2}(0)^{\mathrm{c}}} \Big(\mathcal{E}_{1,1}(x) - \mathcal{E}_{1,2}(x)\Big) \varphi_{\ell_1}(Y_1; x + Y_1(\ell_1))\ \mathrm{d}x \right| \\
&\qquad \le C \int_{B_{r/2}(0)^{\mathrm{c}}} e^{-\widetilde{\gamma}|x|}\ \mathrm{d}x \le C e^{-\widetilde{\gamma} r/4} \int_{B_{r/2}(0)^{\mathrm{c}}} e^{-\widetilde{\gamma}|x|/2}\ \mathrm{d}x \le C e^{-\widetilde{\gamma} r/4}. \qquad (6.66)
\end{aligned}
$$

We estimate (6.63) using Lemma 6.13

$$\begin{aligned}
&\left|\int_{\mathbb{R}^3} \mathcal{E}_{1,2}(x)\Big(\varphi_{\ell_1}(Y_1; x+Y(\ell_1)) - \varphi_{\ell_2}(Y_2; x+Y(\ell_2))\Big)\,\mathrm{d}x\right| \\
&\qquad \le C\int_{\mathbb{R}^3} |\varphi_{\ell_1}(Y_1; x+Y_1(\ell_1)) - \varphi_{\ell_2}(Y_2; x+Y_2(\ell_2))|\,\mathrm{d}x \\
&\qquad \le Ce^{-\widetilde{\gamma}r/4}\int_{\mathbb{R}^3} e^{-\widetilde{\gamma}|x|/2}\,\mathrm{d}x \le Ce^{-\widetilde{\gamma}r/4}.
\end{aligned} \tag{6.67}$$

Collecting the estimates (6.62)–(6.67) gives the first desired result (6.49).

It remains to show (6.50). Let $n_1 \in \Lambda_1'$ satisfy $r_{\ell_1 n_1}(Y_1) \le r$, then by (6.8), there exists unique $n_2 \in \Lambda_2'$ satisfying $Y_1(n_1) - Y_1(\ell_1) = Y_2(n_2) - Y_2(\ell_2)$. Applying (5.89)–(5.90) yields

$$\begin{aligned}
E_{\ell_i,n_i}(Y_i) = &\int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_{1,i}(x)}{\partial Y_i(n_i)}\varphi_{\ell_i}(Y_i; x+Y_i(\ell_i))\,\mathrm{d}x \\
&+ \int_{\mathbb{R}^3} \mathcal{E}_{1,i}(x)\frac{\partial \varphi_{\ell_i}}{\partial Y_i(n_i)}(Y_i; x+Y_i(\ell_i))\,\mathrm{d}x.
\end{aligned} \tag{6.68}$$

Define the first variations

$$\overline{u}_i = \frac{\partial u_i}{\partial Y_i(n_i)}, \quad \overline{\phi}_i = \frac{\partial \phi_i}{\partial Y_i(n_i)}, \quad \overline{m}_i(x) = \frac{\partial m_i}{\partial Y_i(n_i)},$$

which solve the linearised TFW equations (5.24), then

$$\frac{\partial \mathcal{E}_{1,i}}{\partial Y_i(n_i)} = 2\nabla u_i \cdot \nabla \overline{u}_i + \frac{10}{3}u_i^{7/3}\overline{u}_i + \frac{1}{2}\overline{\phi}_i\left(m_i - u_i^2\right) + \frac{1}{2}\phi_i(\overline{m}_i - 2u_i\overline{u}_i).$$

It follows from applying Lemma 5.6 and Proposition 2.1 that for all $x \in \mathbb{R}^3$

$$\begin{aligned}
\left|\frac{\partial \mathcal{E}_{1,i}(x)}{\partial Y_i(n_i)}\right| &\le C\left(|\nabla \overline{u}_i(x)| + |\overline{u}_i(x)| + |\overline{\phi}_i(x)| + |\overline{m}_i(x)|\right) \\
&\le Ce^{-\gamma_0|x+Y_1(\ell_1)-Y_1(n_1)|},
\end{aligned} \tag{6.69}$$

where we have used that $Y_1(\ell_1) - Y_1(n_1) = Y_2(\ell_2) - Y_2(n_2)$.

By (6.68), we decompose the following difference into four terms

$$
\begin{aligned}
&E_{\ell_1,n_1}(Y_1) - E_{\ell_2,n_2}(Y_2) \\
&= \int_{\mathbb{R}^3} \left(\frac{\partial \mathcal{E}_{1,1}(x)}{\partial Y_1(n_1)} - \frac{\partial \mathcal{E}_{1,2}(x)}{\partial Y_2(n_2)} \right) \varphi_{\ell_1}(Y_1; x + Y_1(\ell_1))\, \mathrm{d}x && (6.70)\\
&\quad + \int_{\mathbb{R}^3} \left(\mathcal{E}_{1,1}(x) - \mathcal{E}_{1,2}(x)\right) \frac{\partial \varphi_{\ell_1}}{\partial Y_1(n_1)}(Y_1; x + Y_1(\ell_1))\, \mathrm{d}x && (6.71)\\
&\quad + \int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_{1,2}(x)}{\partial Y_2(n_2)} \left(\varphi_{\ell_1}(Y_1; x + Y_1(\ell_1)) - \varphi_{\ell_2}(Y_2; x + Y_2(\ell_2))\right)\, \mathrm{d}x && (6.72)\\
&\quad + \int_{\mathbb{R}^3} \mathcal{E}_{1,2}(x) \left(\frac{\partial \varphi_{\ell_1}}{\partial Y_1(n_1)}(Y_1; x + Y_1(\ell_1)) - \frac{\partial \varphi_{\ell_2}}{\partial Y_2(n_2)}(Y_2; x + Y_2(\ell_2)) \right)\, \mathrm{d}x. && (6.73)
\end{aligned}
$$

The two terms (6.72)–(6.73) can be estimated directly via Lemma 6.13 and (6.69). We consider (6.72) first, and let $\gamma_1 = \min\{\gamma_0, \frac{\widetilde{\gamma}}{2}, \frac{\gamma'}{4}\}$,

$$
\begin{aligned}
&\left| \int_{\mathbb{R}^3} \frac{\partial \mathcal{E}_{1,2}(x)}{\partial Y_2(n_2)} \left(\varphi_{\ell_1}(Y_1; x + Y_1(\ell_1)) - \varphi_{\ell_2}(Y_2; x + Y_2(\ell_2))\right)\, \mathrm{d}x \right| \\
&\quad \le C \int_{\mathbb{R}^3} e^{-\gamma_0 |x + Y_1(\ell_1) - Y_1(n_1)|} e^{-\widetilde{\gamma}(|x| + r)}\, \mathrm{d}x \\
&\quad \le C \int_{\mathbb{R}^3} e^{-\gamma_1 |x + Y_1(\ell_1) - Y_1(n_1)|} e^{-\widetilde{\gamma}(|x| + r)}\, \mathrm{d}x \le C e^{-\gamma_1 (r + r_{\ell_1 n_1})} \int_{\mathbb{R}^3} e^{-\widetilde{\gamma}|x|/2}\, \mathrm{d}x \\
&\quad = C e^{-\gamma_1 (r + r_{\ell_1 n_1})}.
\end{aligned}
$$

Applying an similar argument to estimate (6.73), we obtain

$$
\begin{aligned}
&\left| \int_{\mathbb{R}^3} \mathcal{E}_{1,2}(x) \left(\frac{\partial \varphi_{\ell_1}}{\partial Y_1(n_1)}(Y_1; x + Y_1(\ell_1)) - \frac{\partial \varphi_{\ell_2}}{\partial Y_2(n_2)}(Y_2; x + Y_2(\ell_2)) \right)\, \mathrm{d}x \right| \\
&\quad \le \int_{\mathbb{R}^3} e^{-\widetilde{\gamma}(|x| + r + r_{\ell_1 n_1})}\, \mathrm{d}x \le C e^{-\widetilde{\gamma}(r + r_{\ell_1 n_1})} \int_{\mathbb{R}^3} e^{-\widetilde{\gamma}|x|}\, \mathrm{d}x \le C e^{-\gamma_1 (r + r_{\ell_1 n_1})}.
\end{aligned}
$$

The remaining two terms (6.70)–(6.71) can be estimated by repeating the decomposition argument (6.64)–(6.66). For (6.71), by following the argument verbatim and applying (5.6c), we deduce

$$\begin{aligned}
&\left|\int_{B_{r/2}(0)}\Big(\mathcal{E}_{1,1}(x)-\mathcal{E}_{1,2}(x)\Big)\frac{\partial\varphi_{\ell_1}}{\partial Y_1(n_1)}(x+Y_1(\ell_1))\,\mathrm{d}x\right|\\
&\quad\le Ce^{-\gamma' r/4}\int_{B_{r/2}(0)}e^{-\widetilde{\gamma}(|x|+|x+Y_1(\ell_1)-Y_1(n_1)|)}\,\mathrm{d}x\\
&\quad\le Ce^{-\gamma' r/4}e^{-\widetilde{\gamma}r_{\ell_1 n_1}/2}\int_{B_{r/2}(0)}e^{-\widetilde{\gamma}|x|/2}\,\mathrm{d}x\le Ce^{-\gamma_1(r+r_{\ell_1 n_1})}.
\end{aligned}$$

Similarly,

$$\begin{aligned}
&\left|\int_{B_{r/2}(0)^{\mathrm{c}}}\Big(\mathcal{E}_{1,1}(x)-\mathcal{E}_{1,2}(x)\Big)\frac{\partial\varphi_{\ell_1}}{\partial Y_1(n_1)}(x+Y_1(\ell_1))\,\mathrm{d}x\right|\\
&\le C\int_{B_{r/2}(0)^{\mathrm{c}}}e^{-\widetilde{\gamma}(|x|+|x+Y_1(\ell_1)-Y_1(n_1)|)}\,\mathrm{d}x\le Ce^{-\widetilde{\gamma}r_{\ell_1 n_1}/4}\int_{B_{r/2}(0)^{\mathrm{c}}}e^{-3\widetilde{\gamma}|x|/4}\,\mathrm{d}x\\
&\le Ce^{-\widetilde{\gamma}(r+r_{\ell_1 n_1})/4}\int_{B_{r/2}(0)^{\mathrm{c}}}e^{-\widetilde{\gamma}|x|/4}\,\mathrm{d}x\le Ce^{-\gamma_1(r+r_{\ell_1 n_1})/2}.
\end{aligned}$$

For the term (6.70), using Lemmas 5.6 and 5.7, we infer

$$\begin{aligned}
&\left|\int_{B_{r/2}(0)}\left(\frac{\partial\mathcal{E}_{1,1}(x)}{\partial Y_1(n_1)}-\frac{\partial\mathcal{E}_{1,2}(x)}{\partial Y_2(n_2)}\right)\varphi_{\ell_1}(Y_1;x+Y_1(\ell_1))\,\mathrm{d}x\right|\\
&\quad\le C\int_{B_{r/2}(0)}e^{-\gamma'(|x+Y_1(\ell_1)-Y_1(n_1)|+3r/4-|x|)}e^{-\widetilde{\gamma}|x|}\,\mathrm{d}x\\
&\quad\le Ce^{-\gamma' r/4}\int_{B_{r/2}(0)}e^{-\gamma_1(|x+Y_1(\ell_1)-Y_1(n_1)|)}e^{-\widetilde{\gamma}|x|}\,\mathrm{d}x\\
&\quad\le Ce^{-\gamma_1(r+r_{\ell_1 n_1})}\int_{B_{r/2}(0)}e^{-\widetilde{\gamma}|x|/2}\,\mathrm{d}x\le Ce^{-\gamma_1(r+r_{\ell_1 n_1})}.
\end{aligned}$$

The final estimate is

$$\begin{aligned}
&\left|\int_{B_{r/2}(0)^{\mathrm{c}}}\left(\frac{\partial\mathcal{E}_{1,1}(x)}{\partial Y_1(n_1)}-\frac{\partial\mathcal{E}_{1,2}(x)}{\partial Y_2(n_2)}\right)\varphi_{\ell_1}(Y_1;x+Y_1(\ell_1))\,\mathrm{d}x\right|\\
&\le C\int_{B_{r/2}(0)^{\mathrm{c}}}e^{-\gamma_1|x+Y_1(\ell_1)-Y_1(n_1)|}e^{-\widetilde{\gamma}|x|}\,\mathrm{d}x\le Ce^{-\gamma_1 r_{\ell_1 n_1}}\int_{B_{r/2}(0)}e^{-\widetilde{\gamma}|x|/2}\,\mathrm{d}x\\
&\le Ce^{-\gamma_1 r_{\ell_1 n_1}}e^{-\widetilde{\gamma}r/4}\le Ce^{-\gamma_1(r+r_{\ell_1 n_1})/2}.
\end{aligned}\tag{6.74}$$

Collecting (6.70)–(6.74) gives the desired estimate (6.50)

$$|E_{\ell_1,n_1}(Y_1) - E_{\ell_2,n_2}(Y_2)| \leq Ce^{-\gamma_1(r+r_{\ell_1 n_1})/2}.$$

□

6.8 Proof of site potential results

In this section, we describe and prove the properties of the site potentials defined in Section 6.3.

Theorem 6.14. *Denote $\Lambda_1 = \Lambda$ and for $\ell \in \Lambda_1$, $V^1_\ell = V_\ell$. Similarly, denote $\Lambda_2 = \Lambda^{\text{hom}}$ and for $\ell \in \Lambda_2$, $V^2_\ell = V^{\text{hom}}$, defined in (6.12). For $k = 1, 2$, the site potential V^k_ℓ satisfy the following properties* **(V)***: Let $U \in \dot{\mathscr{W}}^{1,2}(\Lambda_k, \lambda)$.*

(V.R) *Regularity: At each $\ell \in \Lambda_k$, V^k_ℓ possesses all partial derivative, denoted by $V^k_{\ell,\boldsymbol{\rho}}(DU(\ell))$, $\boldsymbol{\rho} \in (\Lambda_k - \ell)^j$ for $j \in \mathbb{N}$.*

(V.L) *Locality: There exists $\gamma > 0$ such that for all $j \in \mathbb{N}$ and $\ell \in \Lambda_k$, $\boldsymbol{\rho} = (\rho_1, \ldots, \rho_j) \in (\Lambda_k - \ell)^j$*

$$|V^k_{\ell,\boldsymbol{\rho}}(DU(\ell))| \leq C_j e^{-\gamma \sum_{i=1}^{j} |\rho_i|},$$

where $C_j = C_j(\lambda), \gamma = \gamma(\lambda)$.

(V.H) *Homogeneity: Let $Y_1, Y_2 \in \mathscr{A}(\Lambda, \lambda) \cup \mathscr{A}(\Lambda^{\text{hom}}, \lambda)$ and for $i = 1, 2$, let $\Lambda'_i = \text{Dom}(Y_i)$ and $j_i = 1$ if $\Lambda'_i = \Lambda$, otherwise let $j_i = 2$. In addition, let $U_i \in \dot{\mathscr{W}}^{1,2}(\Lambda'_i, \lambda)$ denote the displacement corresponding to Y_i. There exist $C = C(\lambda'), \gamma = \gamma(\lambda') > 0$ such that for any $\ell_1 \in \Lambda'_1, \ell_2 \in \Lambda'_2$ and $r \geq 0$ satisfying*

$$\{Y_1(n) - Y_1(\ell_1) \mid r_{\ell_1 n}(Y_1) \leq r\} = \{Y_2(n) - Y_2(\ell_2) \mid r_{\ell_2 n}(Y_2) \leq r\},$$

then

$$\left|V^{j_1}_{\ell_1}(DU_1(\ell_1)) - V^{j_2}_{\ell_2}(DU_2(\ell_2))\right| \leq Ce^{-\gamma r}. \tag{6.75}$$

Additionally, there exists a function $V^{\mathrm{hom}} : D(\Lambda^{\mathrm{hom}}) \to \mathbb{R}$ *such that for all* $U^{\mathrm{hom}} \in \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})$ *and* $\ell \in \Lambda^{\mathrm{hom}}$, $V_\ell^{\mathrm{hom}}(DU^{\mathrm{hom}}(\ell)) = V^{\mathrm{hom}}(DU^{\mathrm{hom}}(\ell))$.

Moreover, there exist $C_1 > 0$, $C = C(\lambda'), \gamma = \gamma(\lambda') > 0$ *and such that for any* $U \in \dot{\mathscr{W}}^{1,2}(\Lambda, \lambda)$, $\ell \in \Lambda^{\mathrm{hom}} \setminus B_{R_{\mathrm{def}}}$ *and* $\rho \in \Lambda - \ell$ *satisfying* $|\rho| < \frac{|\ell| - R_{\mathrm{def}} - C_1\lambda^2}{2}$

$$\left|V^{\mathrm{hom}}(DI^{\mathrm{hom}}U(\ell)) - V_\ell(DU(\ell))\right| \le Ce^{-\gamma|\ell|}, \tag{6.76}$$

$$\left|V^{\mathrm{hom}}_{,\rho}(DI^{\mathrm{hom}}U(\ell)) - V_{\ell,\rho}(DU(\ell))\right| \le Ce^{-\gamma(|\ell|+|\rho|)}. \tag{6.77}$$

Similarly, there exist $C_1 > 0$, $C = C(\lambda'), \gamma = \gamma(\lambda') > 0$ *and such that for any* $U^{\mathrm{hom}} \in \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}}, \lambda)$, $\ell \in \Lambda^{\mathrm{hom}} \setminus B_{R_{\mathrm{def}}}$ *and* $\rho \in \Lambda^{\mathrm{hom}}_*$ *satisfying* $|\rho| < \frac{|\ell| - R_{\mathrm{def}} - C_1\lambda^2}{2}$

$$\left|V^{\mathrm{hom}}(DU^{\mathrm{hom}}(\ell)) - V_\ell(DI^{\mathrm{def}}U^{\mathrm{hom}}(\ell))\right| \le Ce^{-\gamma|\ell|}, \tag{6.78}$$

$$\left|V^{\mathrm{hom}}_{,\rho}(DU^{\mathrm{hom}}(\ell)) - V_{\ell,\rho}(DI^{\mathrm{def}}U^{\mathrm{hom}}(\ell))\right| \le Ce^{-\gamma(|\ell|+|\rho|)}. \tag{6.79}$$

The constant C_1 *appearing above is independent of* λ *and* λ'.

We remark that the statement of **(V.H)** uses the constant $\lambda' > 0$ defined from $\lambda > 0$ in Remark 24.

Proof of Theorem 6.14. For $\ell \in \Lambda$, recall the definition (6.10) of the site potential V_ℓ. It follows from **(SE)** that V_ℓ inherits the properties of the site energy. Let $U \in \dot{\mathscr{W}}^{1,2}(\Lambda, \lambda)$ and define $Y = Y_0 + U \in \mathscr{A}(\Lambda, \lambda)$.

In particular, the site potential inherits its regularity from **(SE.R)**: for all $\ell \in \Lambda$ and $U \in \dot{\mathscr{W}}^{1,2}(\Lambda)$, $V_\ell(DU(\ell))$ possess all partial derivatives, so **(V.R)** holds. We also obtain locality from **(SE.L)**: there exists $\gamma > 0$ such that for all $j \in \mathbb{N}$, $\ell \in \Lambda$ and $\boldsymbol{\rho} = (\rho_1, \cdots, \rho_j) \in (\Lambda - \ell)^j$

$$|V_{\ell,\boldsymbol{\rho}}(DU(\ell))| \le C_j e^{-\gamma \sum_{i=1}^j |Y(\ell+\rho_i) - Y(\ell)|}.$$

Then applying Lemma 6.8 we deduce

$$|V_{\ell,\boldsymbol{\rho}}(DU(\ell))| \le C'_j e^{-\gamma' \sum_{i=1}^j |\rho_i|},$$

where the constants $C'_j, \gamma' > 0$ depend only on λ, hence **(V.L)** holds for V_ℓ. An identical argument shows that V_ℓ^{hom} satisfies **(V.R)**, **(V.L)**.

We now show **(V.H)** and remark that the estimate (6.75) follows directly from **(SE.H)**. To show (6.76)–(6.77), let $U \in \dot{\mathscr{W}}^{1,2}(\Lambda, \lambda)$ and define $Y = Y_0 + U \in \mathscr{A}(\Lambda, \lambda)$. Recall Lemma 6.10, which states that $I^{\mathrm{hom}}U(\ell) = U(\ell)$ for $\ell \in \Lambda \setminus B_{R_{\mathrm{def}}}$ hence applying **(SE.H)** with $r = \max\{|\ell| - R_{\mathrm{def}}, 0\}$ implies (6.76) and

$$\left|V^{\mathrm{hom}}_{,\rho}(DI^{\mathrm{hom}}U(\ell)) - V_{\ell,\rho}(DU(\ell))\right| \le Ce^{-\gamma(|\ell|+|\rho|)},$$

for all $\rho \in \Lambda - \ell$ satisfying $|Y(\ell+\rho) - Y(\ell)| \le |\ell| - R_{\mathrm{def}}$. It remains to show there exists $C_1 > 0$ such that $|\rho| \le \frac{|\ell| - R_{\mathrm{def}} - C_1\lambda^2}{2}$ implies $|Y(\ell+\rho) - Y(\ell)| \le |\ell| - R_{\mathrm{def}}$.

Applying the estimate (6.28) from the proof of Lemma 6.8 and Young's inequality, we deduce

$$\begin{aligned} |Y(\ell+\rho) - Y(\ell)| = |\rho + D_\rho U(\ell)| \le |\rho| + |D_\rho U(\ell)| &\le |\rho| + C_0^{1/2}\|DU\|_{\ell^2}|\rho|^{1/2} \\ &\le |\rho| + C_0^{1/2}\lambda|\rho|^{1/2} \le 2|\rho| + \frac{C_0\lambda^2}{4}. \end{aligned} \tag{6.80}$$

Let $C_1 = \frac{C_0}{4} > 0$, then for $|\rho| \le \frac{|\ell| - R_{\mathrm{def}} - C_1\lambda^2}{2}$, it follows from (6.80) that

$$|Y(\ell+\rho) - Y(\ell)| \le 2|\rho| + C_1\lambda^2 \le |\ell| - R_{\mathrm{def}},$$

hence (6.77) holds. An identical argument, using Lemma 6.11, shows that the estimates (6.78)–(6.79) hold. $\square$

6.9 Proof of energy difference functional results

This section is dedicated to the proof of Theorem 6.4, which states that the energy-difference functionals $\mathscr{E}, \mathscr{E}^{\mathrm{hom}}$ defined in Section 6.4 are defined on $\dot{\mathscr{W}}^{1,2}(\Lambda)$ and $\dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})$, respectively.

Theorem 6.15. *Denote $\Lambda_1 = \Lambda, \Lambda_2 = \Lambda^{\mathrm{hom}}$ and $\mathscr{E}_1 = \mathscr{E}, \mathscr{E}_2 = \mathscr{E}^{\mathrm{hom}}$.*

If the properties **(V)** *are satisfied, then for $i = 1, 2$*

(i) For every $U \in \dot{\mathscr{W}}^{c}(\Lambda_i)$, the sum that formally defines $\mathscr{E}_i(U)$ converges, hence one can rigorously define $\mathscr{E}_i : \dot{\mathscr{W}}^{c}(\Lambda_i) \to \mathbb{R}$.

Moreover, if $\delta\mathscr{E}_i(0)$ is a bounded linear functional on $(\dot{\mathscr{W}}^{c}(\Lambda_i), \|D\cdot\|_{\ell^2(\Lambda_i)})$, then

(ii) $\mathscr{E}_i : \dot{\mathscr{W}}^{c}(\Lambda_i) \to \mathbb{R}$ is continuous with respect to $\|D\cdot\|_{\ell^2(\Lambda_i)}$, hence there exists a unique continuous extension to $\dot{\mathscr{W}}^{1,2}(\Lambda_i)$, which we continue to denote by $\mathscr{E}_i$.

(iii) $\mathscr{E}_i : \dot{\mathscr{W}}^{1,2}(\Lambda_i) \to \mathbb{R}$ is infinitely differentiable.

Due to the length of the argument and the techniques involved, we postpone proving that $\delta\mathscr{E}(0)$ is well-defined on $\dot{\mathscr{W}}^{c}(\Lambda)$.

Remark 25. For $j = 1, 2, 3$, $U \in \dot{\mathscr{W}}^{1,2}(\Lambda)$ and $\boldsymbol{V} = (V_1, \cdots, V_j) \in \big(\dot{\mathscr{W}}^{1,2}(\Lambda)\big)^j$, the j-th variation of $\mathscr{E}$ is given by

$$\langle \delta^j \mathscr{E}(U), \boldsymbol{V}\rangle = \sum_{\ell\in\Lambda} \sum_{\boldsymbol{\rho}\in(\Lambda-\ell)^j} \big\langle V_{\ell,\boldsymbol{\rho}}\big(DU(\ell)\big), D_{\boldsymbol{\rho}} \otimes \boldsymbol{V}(\ell)\big\rangle, \tag{6.81}$$

where $\boldsymbol{\rho} = (\rho_1, \cdots, \rho_j) \in (\Lambda-\ell)^j$ and $D_{\boldsymbol{\rho}} \otimes \boldsymbol{V}(\ell) := \big(D_{\rho_1}V_1(\ell), \cdots, D_{\rho_j}V_j(\ell)\big)$.

Proof of Theorem 6.15. We first prove the results (i) for $\mathscr{E}$ and remark that the proof for $\mathscr{E}^{\rm hom}$ is identical.

(i) Let $U \in \dot{\mathscr{W}}^{c}(\Lambda)$, then there exists $R > 0$ such that U is a constant on $\Lambda\backslash B_R$. We have

$$\mathscr{E}(U) = \sum_{\ell\in\Lambda\cap B_{2R}} \Big(V_\ell\big(DU(\ell)\big) - V_\ell(0)\Big) + \sum_{\ell\in\Lambda\backslash B_{2R}} \Big(V_\ell\big(DU(\ell)\big) - V_\ell(0)\Big).$$

The first term is a finite sum and the second part can be estimated by using **(V.H)**:

$$\sum_{\ell\in\Lambda\backslash B_{2R}} \Big(V_\ell\big(DU(\ell)\big) - V_\ell(0)\Big) \le C \sum_{\ell\in\Lambda\backslash B_{2R}} e^{-\gamma(|\ell|-R)} < \infty. \tag{6.82}$$

Therefore, the energy difference functional $\mathscr{E}$ is well defined on $\dot{\mathscr{W}}^{c}(\Lambda)$.

Suppose that $\delta\mathscr{E}(0)$ is a bounded linear functional on $\dot{\mathscr{W}}^{c}(\Lambda)$. Following this argument verbatim also shows that (ii)–(iii) hold for $\mathscr{E}^{\rm hom}$.

(ii) For $U, V \in \dot{\mathscr{W}}^{\mathrm{c}}(\Lambda)$, we first show that the series

$$\sum_{\ell\in\Lambda} \big\langle \delta V_\ell\big(DU(\ell)\big), DV(\ell)\big\rangle := \sum_{\ell\in\Lambda}\sum_{\rho\in\Lambda-\ell} V_{\ell,\rho}(DU(\ell)) \cdot D_\rho V(\ell) \tag{6.83}$$

is well-defined and then prove this is the Fréchet derivative $\langle \delta\mathscr{E}(U), V\rangle$. Consider the difference

$$\sum_{\ell\in\Lambda} \big\langle \delta V_\ell\big(DU(\ell)\big), DV(\ell)\big\rangle - \langle \delta\mathscr{E}(0), V\rangle = \sum_{\ell\in\Lambda} \big\langle \delta V_\ell\big(DU(\ell)\big) - \delta V_\ell\big(0\big), DV(\ell)\big\rangle\,,$$

then using **(V.R)**, **(V.L)** and Lemma 6.9, we deduce

$$\begin{aligned}
&\Big|\sum_{\ell\in\Lambda} \big\langle \delta V_\ell\big(DU(\ell)\big) - \delta V_\ell\big(0\big), DV(\ell)\big\rangle\Big| \\
&\le \int_0^1 \sum_{\ell\in\Lambda} \big|\big\langle \delta^2 V_\ell(tDU(\ell))DU(\ell), DV(\ell)\big\rangle\big| \,\mathrm{d}t \\
&\le \int_0^1 \sum_{\ell\in\Lambda}\sum_{\rho,\sigma\in\Lambda-\ell} |V_{\ell,\rho\sigma}(tDU(\ell))||D_\rho U(\ell)||D_\sigma V(\ell)| \,\mathrm{d}t \\
&\le C\sum_{\ell\in\Lambda}\sum_{\rho,\sigma\in\Lambda-\ell} e^{-\gamma(|\rho|+|\sigma|)}|D_\rho U(\ell)||D_\sigma V(\ell)| \\
&= C\sum_{\ell\in\Lambda} |DU(\ell)|_\gamma |DV(\ell)|_\gamma \le C\|DU\|_{\ell^2_\gamma}\|DV\|_{\ell^2_\gamma} \le C\|DU\|_{\ell^2}\|DV\|_{\ell^2}.
\end{aligned} \tag{6.84}$$

As we suppose that $\delta\mathscr{E}(0)$ is bounded linear function on $\dot{\mathscr{W}}^{\mathrm{c}}(\Lambda)$, the series (6.83) is well-defined. Consider the difference

$$\begin{aligned}
&\mathscr{E}(U+V) - \mathscr{E}(U) - \sum_{\ell\in\Lambda} \big\langle \delta V_\ell\big(DU(\ell)\big), DV(\ell)\big\rangle \\
&= \sum_{\ell\in\Lambda}\Big(V_\ell\big(D(U+V)(\ell)\big) - V_\ell\big(DU(\ell)\big) - \big\langle \delta V_\ell\big(DU(\ell)\big), DV(\ell)\big\rangle \Big),
\end{aligned}$$

which is well-defined. We now estimate the right-hand term

$$
\begin{aligned}
&\Big|\sum_{\ell\in\Lambda}\Big(V_\ell(D(U+V)(\ell)) - V_\ell(DU(\ell)) - \big\langle \delta V_\ell\big(DU(\ell)\big), DV(\ell)\big\rangle\Big)\Big| \\
&\quad\le \int_0^1 \sum_{\ell\in\Lambda} \big|\big\langle \delta^2 V_\ell\big(D(U+tV)(\ell)\big)DU(\ell), DV(\ell)\big\rangle\big| \ \mathrm{d}t \\
&\quad\le C\|DU\|_{\ell^2}\|DV\|_{\ell^2}, \qquad (6.85)
\end{aligned}
$$

We remark that the constants appearing in (6.84)–(6.85) depend on $\lambda = \sup_{t\in[0,1]}\|DU + tDV\|_{\ell^2(\Lambda)}$. It follows from (6.85) that $\mathscr{E}$ is Fréchet differentiable and hence is continuous for all $U \in \dot{\mathscr{W}}^{\mathrm{c}}(\Lambda)$. Consequently, we uniquely extend $\mathscr{E}$ to $\dot{\mathscr{W}}^{1,2}(\Lambda)$ and remark that the argument (6.83)–(6.85) also shows that $\mathscr{E}$ is Fréchet differentiable on $\dot{\mathscr{W}}^{1,2}(\Lambda)$.

(iii) For $U \in \dot{\mathscr{W}}^{1,2}(\Lambda,\lambda)$ and $j\in\mathbb{N}$ satisfying $j\ge 2$, let $\boldsymbol{V} = (V_1,\cdots,V_j) \in \big(\dot{\mathscr{W}}^{1,2}(\Lambda)\big)^j$ and $\boldsymbol{\rho} = (\rho_1,\cdots,\rho_j)\in(\Lambda-\ell)^j$, by **(V.L)**

$$
\begin{aligned}
&\sum_{\ell\in\Lambda}\sum_{\boldsymbol{\rho}\in(\Lambda-\ell)^j} \big|\big\langle V_{\ell,\boldsymbol{\rho}}\big(DU(\ell)\big), D_{\boldsymbol{\rho}}\otimes\boldsymbol{V}(\ell)\big\rangle\big| \\
&\quad\le \sum_{\ell\in\Lambda}\sum_{\rho_1,\cdots,\rho_j} \big|V_{\ell,\rho_1,\cdots,\rho_j}\big(DU(\ell)\big)\big| \prod_{1\le m\le j}|D_{\rho_m}V_m(\ell)| \\
&\quad\le C\sum_{\ell\in\Lambda}\sum_{\rho_1,\cdots,\rho_j} e^{-\gamma\sum_{i=1}^j-\gamma|\rho_i|}\prod_{1\le m\le j}|D_{\rho_m}V_m(\ell)| \\
&\quad= C\sum_{\ell\in\Lambda}\prod_{1\le i\le j}\Big(\sum_{\rho_i\in\Lambda-\ell} e^{-\gamma|\rho_i|}|D_{\rho_i}V_i(\ell)|\Big) = C\sum_{\ell\in\Lambda}\prod_{1\le i\le j}|DV_i(\ell)|_\gamma. \qquad (6.86)
\end{aligned}
$$

As $j\ge 2$, it follows that $\ell^j\subseteq\ell^2$, hence applying the generalised version of Hölder's inequality to (6.86) gives

$$
\begin{aligned}
&\sum_{\ell\in\Lambda}\sum_{\boldsymbol{\rho}\in(\Lambda-\ell)^j} \big|\big\langle V_{\ell,\boldsymbol{\rho}}\big(DU(\ell)\big), D_{\boldsymbol{\rho}}\otimes\boldsymbol{V}(\ell)\big\rangle\big| \\
&\le C\sum_{\ell\in\Lambda}\prod_{1\le i\le j}|DV_i(\ell)|_\gamma \le C\prod_{1\le i\le j}\Big(\sum_{\ell\in\Lambda}|DV_i(\ell)|_\gamma^j\Big)^{1/j} \\
&\le C\prod_{1\le i\le j}\Big(\sum_{\ell\in\Lambda}|DV_i(\ell)|_\gamma^2\Big)^{1/2} = C\prod_{1\le i\le j}\|DV_i\|_{\ell^2_\gamma} \le C\prod_{1\le i\le j}\|DV_i\|_{\ell^2}. \qquad (6.87)
\end{aligned}
$$

We remark that the constants appearing in (6.86)–(6.87) depend only on λ.

We now show that for all $j \in \mathbb{N}$, $U \in \dot{\mathscr{W}}^{1,2}(\Lambda)$ and $\boldsymbol{V} = (V_1, \cdots, V_j) \in \big(\dot{\mathscr{W}}^{1,2}(\Lambda)\big)^j$, that $\mathscr{E}$ is j-times differentiable and

$$\begin{aligned} \langle \delta^j \mathscr{E}(U), \boldsymbol{V} \rangle &= \sum_{\ell \in \Lambda} \sum_{\boldsymbol{\rho} \in (\Lambda - \ell)^j} \big\langle V_{\ell,\boldsymbol{\rho}}\big(DU(\ell)\big), D_{\boldsymbol{\rho}} \otimes \boldsymbol{V}(\ell) \big\rangle \\ &=: \sum_{\ell \in \Lambda} \big\langle \delta^j V_\ell\big(DU(\ell)\big), D \otimes \boldsymbol{V}(\ell) \big\rangle , \end{aligned} \tag{6.88}$$

where $D \otimes \boldsymbol{V}(\ell) = (DV_1(\ell), \ldots, DV_j(\ell))$. We argue by induction, and observe that the estimate (6.85) shows (6.88) holds when $j = 1$, so we now consider the induction step, for $j \in \mathbb{N}$. Let $V \in \dot{\mathscr{W}}^{1,2}(\Lambda)$ and define $V_{j+1} = V_j$ and $\boldsymbol{V}' = (V_1, \ldots, V_{j+1}) \in (\dot{\mathscr{W}}^{1,2}(\Lambda))^{j+1}$, then

$$\begin{aligned} &\Big| \big\langle \delta^j \mathscr{E}(U + V) - \delta^j \mathscr{E}(U), \boldsymbol{V} \big\rangle - \sum_{\ell \in \Lambda} \big\langle \delta^{j+1} V_\ell\big(DU(\ell)\big), D \otimes \boldsymbol{V}'(\ell) \big\rangle \Big| \\ &= \Big| \sum_{\ell \in \Lambda} \big\langle \delta^j V_\ell\big(D(U+V)(\ell)\big) - \delta^j V_\ell\big(DU(\ell)\big) - \delta^{j+1} V_\ell\big(DU(\ell)\big) DV(\ell), D\boldsymbol{V}(\ell) \big\rangle \Big| \\ &\leq \int_0^1 \sum_{\ell \in \Lambda} \big| \big\langle \delta^{j+2} V_\ell\big(D(U + tV)(\ell)\big) DU(\ell), D \otimes \boldsymbol{V}'(\ell) \big\rangle \big| \, \mathrm{d}t \\ &\leq C \|DU\|_{\ell^2(\Lambda)} \prod_{1 \leq i \leq j+1} \|DV_i\|_{\ell^2(\Lambda)}, \end{aligned}$$

where have applied (6.87) to obtain the final estimate. This completes the induction argument, hence $\mathscr{E}$ is infinitely differentiable. □

We remark that the estimate (6.86) will be used to prove Lemma 6.21.

It remains to show that $\delta \mathscr{E}(0)$ and $\delta \mathscr{E}^{\mathrm{hom}}(0)$ are bounded linear functionals on $\dot{\mathscr{W}}^{\mathrm{c}}(\Lambda)$ and $\dot{\mathscr{W}}^{\mathrm{c}}(\Lambda^{\mathrm{hom}})$, respectively.

Lemma 6.16. *$\delta \mathscr{E}^{\mathrm{hom}}(0) = 0$ on $\dot{\mathscr{W}}^{\mathrm{c}}(\Lambda^{\mathrm{hom}})$, in particular it is a bounded linear functional.*

This result ensures that $\mathscr{E}^{\mathrm{hom}}$ satisfies the regularity properties given in Theorem 6.15.

Proof of Lemma 6.16. This result follows directly from [56, Lemma 2.12], once we establish that for any $U \in \dot{\mathscr{W}}^{\mathrm{c}}(\Lambda^{\mathrm{hom}})$, the sum

$$\sum_{\ell \in \Lambda} \sum_{\rho \in \Lambda_*^{\mathrm{hom}}} V_{,\rho}^{\mathrm{hom}}(0) \cdot D_\rho U(\ell) \tag{6.89}$$

is well-defined.

As $U \in \dot{\mathscr{W}}^{\mathrm{c}}(\Lambda^{\mathrm{hom}})$, U is constant outside $B_R(0)$, for some $R > 0$. Fix $\rho \in \Lambda_*^{\mathrm{hom}}$, then following the proof of Lemma 6.6 for each $\ell \in \Lambda^{\mathrm{hom}}$, there exists a path of lattice points $\mathscr{P}^{\mathrm{hom}}(\ell, \ell+\rho) := \{\ell_i\}_{1 \le i \le N_\rho + 1} \subset \Lambda^{\mathrm{hom}}$, such that for each $1 \le i \le N_\rho$, $\ell_{i+1} \in \mathscr{N}(\ell_i)$ and $N_\rho \le C'|\rho|$, where $C' > 0$ is independent of ℓ and ρ. In addition, these paths are translation invariant, that is for all $\ell \in \Lambda^{\mathrm{hom}}$, $\mathscr{P}^{\mathrm{hom}}(\ell, \ell+\rho) = \ell + \mathscr{P}^{\mathrm{hom}}(0, \rho)$. Then, applying this path decomposition yields

$$\begin{aligned} \sum_{\ell \in \Lambda^{\mathrm{hom}}} |D_\rho U(\ell)| &\le \sum_{\ell \in \Lambda^{\mathrm{hom}}} \sum_{i=1}^{N_\rho} |D_{\rho_i} U(\ell_i)| \le \sum_{\ell \in \Lambda^{\mathrm{hom}}} \sum_{i=1}^{N_\rho} \sum_{\rho' \in \mathscr{N}(\ell_i) - \ell_i} |D_{\rho'} U(\ell_i)| \\ &\le \sum_{\ell' \in \Lambda^{\mathrm{hom}}} \sum_{\rho' \in \mathscr{N}(\ell') - \ell'} |D_{\rho'} U(\ell')| \left| \left\{ \ell \in \Lambda^{\mathrm{hom}} \,\middle|\, \ell' \in \mathscr{P}(\ell, \ell+\rho) \right\} \right|. \end{aligned} \tag{6.90}$$

We apply the translation invariance property of the paths to estimate

$$\begin{aligned} \left| \left\{ \ell \in \Lambda^{\mathrm{hom}} \,\middle|\, \ell' \in \mathscr{P}(\ell, \ell+\rho) \right\} \right| &= \left| \left\{ \ell \in \Lambda^{\mathrm{hom}} \,\middle|\, \ell \in -\ell' + \mathscr{P}(0, \rho) \right\} \right| \\ &= |\mathscr{P}(0, \rho)| \le C'|\rho|. \end{aligned} \tag{6.91}$$

Inserting (6.91) into (6.90) yields

$$\sum_{\ell \in \Lambda^{\mathrm{hom}}} |D_\rho U(\ell)| \le C|\rho| \sum_{\ell \in \Lambda^{\mathrm{hom}}} \sum_{\rho' \in \mathscr{N}(\ell') - \ell'} |D_{\rho'} U(\ell')|.$$

Moreover, there exists $R' > 0$ such that $\mathscr{N}(\ell) - \ell \subset B_{R'}(0)$ for all $\ell \in \Lambda^{\mathrm{hom}}$, hence for $\ell \in \Lambda^{\mathrm{hom}} \cap B_{R+R'}(0)^{\mathrm{c}}$ and $\rho' \in \mathscr{N}(\ell) - \ell$, $D_{\rho'} U(\ell) = 0$. Consequently, applying Cauchy–Schwarz, we deduce

$$\begin{aligned}
\sum_{\ell\in\Lambda^{\mathrm{hom}}} |D_\rho U(\ell)| &\le C|\rho| \sum_{\ell\in\Lambda^{\mathrm{hom}}\cap B_{R+R'}(0)} \sum_{\rho'\in\mathscr{N}(\ell)-\ell} |D_{\rho'}U(\ell)| \\
&\le C|\rho|(R+R')^{3/2}\left(\sum_{\ell\in\Lambda^{\mathrm{hom}}\cap B_{R+R'}(0)}\left(\sum_{\rho'\in\mathscr{N}(\ell)-\ell}|D_{\rho'}U(\ell)|\right)^2\right)^{1/2} \\
&\le C|\rho|(R+R')^{3/2}\left(\sum_{\ell\in\Lambda^{\mathrm{hom}}\cap B_{R+R'}(0)}\sum_{\rho'\in\mathscr{N}(\ell)-\ell}|D_{\rho'}U(\ell)|^2\right)^{1/2} \\
&= C|\rho|(R+R')^{3/2}\|DU\|_{\ell^2(\Lambda^{\mathrm{hom}})}, \qquad (6.92)
\end{aligned}$$

where the constant C is independent of ρ. Applying **(V.L)** and (6.92), we deduce

$$\begin{aligned}
&\sum_{\rho\in\Lambda_*^{\mathrm{hom}}}\sum_{\ell\in\Lambda^{\mathrm{hom}}} |V_{,\rho}^{\mathrm{hom}}(0)\cdot D_\rho U(\ell)| \\
&\quad\le C\sum_{\rho\in\Lambda_*^{\mathrm{hom}}} e^{-\gamma|\rho|}\sum_{\ell\in\Lambda^{\mathrm{hom}}}|D_\rho U(\ell)| \\
&\quad\le C(R+R')^{3/2}\|DU\|_{\ell^2(\Lambda^{\mathrm{hom}})}\sum_{\rho\in\Lambda_*^{\mathrm{hom}}}|\rho|e^{-\gamma|\rho|}<\infty. \qquad (6.93)
\end{aligned}$$

As the sum (6.93) converges, changing the order of summation of (6.89) is allowed and the sum is well-defined. Then as $U\in\dot{\mathscr{W}}^{\mathrm{c}}(\Lambda^{\mathrm{hom}})$, it follows that for all $\rho\in\Lambda_*^{\mathrm{hom}}$, $\sum_{\ell\in\Lambda^{\mathrm{hom}}} D_\rho U(\ell)=0$, hence the desired result holds

$$\langle\delta\mathscr{E}^{\mathrm{hom}}(0),U\rangle = \sum_{\rho\in\Lambda_*^{\mathrm{hom}}} V_{,\rho}^{\mathrm{hom}}(0)\sum_{\ell\in\Lambda^{\mathrm{hom}}} D_\rho U(\ell) = 0.$$

□

In order to show that $\delta\mathcal{E}(0)$ is a well-defined operator on $\dot{\mathscr{W}}^{\mathrm{c}}(\Lambda)$, we use the interpolation operators $I^{\mathrm{hom}}, I^{\mathrm{def}}$ to compare displacements on Λ to those on Λ^{hom} and vice versa. In fact, we show the more general result.

Lemma 6.17. *The operator $\delta\mathscr{E}(0)$ is a bounded linear operator on $\dot{\mathscr{W}}^{\mathrm{c}}(\Lambda)$. It follows that $\mathscr{E}$ can be extended to $\dot{\mathscr{W}}^{1,2}(\Lambda)$ and is infinitely differentiable.*

Recall the interpolation functions $I^{\mathrm{hom}}:\dot{\mathscr{W}}^{1,2}(\Lambda)\to\dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})$,

$I^{\mathrm{def}} : \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}}) \to \dot{\mathscr{W}}^{1,2}(\Lambda)$ defined in Lemmas 6.10 and 6.11. Then for all $U \in \dot{\mathscr{W}}^{1,2}(\Lambda, \lambda)$:

1. *for all $V \in \dot{\mathscr{W}}^{1,2}(\Lambda)$*

$$|\langle \delta\mathcal{E}(U), V\rangle - \langle \delta\mathcal{E}^{\mathrm{hom}}(I^{\mathrm{hom}}U), I^{\mathrm{hom}}V\rangle| \leq C\|DV\|_{\ell^2(\Lambda)}, \tag{6.94}$$

   where $C > 0$ depends on $\|I^{\mathrm{hom}}\|_{\dot{\mathscr{W}}^{1,2}(\Lambda),\dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})}$ and $\lambda' > 0$.

2. *for all $V^{\mathrm{hom}} \in \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})$*

$$|\langle \delta\mathcal{E}(U), I^{\mathrm{def}}V^{\mathrm{hom}}\rangle - \langle \delta\mathcal{E}^{\mathrm{hom}}(I^{\mathrm{hom}}U), V^{\mathrm{hom}}\rangle| \leq C\|DV^{\mathrm{hom}}\|_{\ell^2(\Lambda^{\mathrm{hom}})}, \tag{6.95}$$

   where $C > 0$ depends on $\|I^{\mathrm{def}}\|_{\dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}}),\dot{\mathscr{W}}^{1,2}(\Lambda)}$ and $\lambda' > 0$.

Remark 26. The parameter $\lambda' > 0$ is introduced in (6.40) of Remark 24. Moreover, this remark explains why the constants appearing in Lemma 6.17 depend on λ' instead of λ. $\square$

Proof of Lemma 6.17. We first show that $\delta\mathscr{E}(0)$ is a bounded linear operator on $\dot{\mathscr{W}}^{\mathrm{c}}(\Lambda)$. A slight generalisation allows us to also prove (6.94), which is more general, so we prove the more general result.

Let $r = 2R_{\mathrm{def}} > 0$, $U \in \dot{\mathscr{W}}^{\mathrm{c}}(\Lambda, \lambda), V \in \dot{\mathscr{W}}^{\mathrm{c}}(\Lambda)$ and observe that for $\ell \in \Lambda^{\mathrm{hom}} \setminus B_{R_{\mathrm{def}}}$ and $\rho \in \Lambda^{\mathrm{hom}} \setminus B_{R_{\mathrm{def}}} - \ell$, that

$$D_\rho I^{\mathrm{hom}}V(\ell) = I^{\mathrm{hom}}V(\ell+\rho) - I^{\mathrm{hom}}V(\ell) = V(\ell+\rho) - V(\ell) = D_\rho V(\ell).$$

It follows from the triangle inequality that for $\ell \in \Lambda^{\mathrm{hom}} \setminus B_r$ and either $\rho \in \Lambda_*^{\mathrm{hom}} \cap B_{R_{\mathrm{def}}}$ or $\rho \in \left(\Lambda^{\mathrm{hom}} \setminus B_{R_{\mathrm{def}}}\right) - \ell$, that $D_\rho I^{\mathrm{hom}}V(\ell) = D_\rho V(\ell)$. Moreover, as $\Lambda \setminus B_{R_{\mathrm{def}}} = \Lambda^{\mathrm{hom}} \setminus B_{R_{\mathrm{def}}}$ it also follows that

$$\begin{aligned}
(\Lambda \setminus B_r) \times ((\Lambda - \ell) \cap B_{R_{\mathrm{def}}}) &= \left(\Lambda^{\mathrm{hom}} \setminus B_r\right) \times \left(\Lambda_*^{\mathrm{hom}} \cap B_{R_{\mathrm{def}}}\right), \\
(\Lambda \setminus B_r) \times ((\Lambda \setminus B_{R_{\mathrm{def}}}) - \ell) &= \left(\Lambda^{\mathrm{hom}} \setminus B_r\right) \times \left(\left(\Lambda^{\mathrm{hom}} \setminus B_{R_{\mathrm{def}}}\right) - \ell\right).
\end{aligned}$$

We decompose the following difference into four terms

$$
\begin{aligned}
&\sum_{\ell_1\in\Lambda}\big\langle\delta V_{\ell_1}\big(DU(\ell_1)\big),DV(\ell_1)\big\rangle-\big\langle\delta\mathscr{E}^{\mathrm{hom}}(I^{\mathrm{hom}}U),DI^{\mathrm{hom}}V\big\rangle\\
&=\sum_{\ell_1\in\Lambda}\sum_{\rho_1\in\Lambda-\ell_1}V_{\ell_1,\rho_1}(DU(\ell_1))\cdot D_{\rho_1}V(\ell_1)\\
&\qquad\qquad-\sum_{\ell_2\in\Lambda^{\mathrm{hom}}}\sum_{\rho_2\in\Lambda_*^{\mathrm{hom}}}V^{\mathrm{hom}}_{,\rho_2}(DI^{\mathrm{hom}}U(\ell_2))\cdot D_{\rho_2}I^{\mathrm{hom}}V(\ell_2)\\
&=\sum_{\substack{\ell\in\Lambda^{\mathrm{hom}}\\|\ell|\ge r}}\sum_{\substack{\rho\in\Lambda_*^{\mathrm{hom}}\\|\rho|<R_{\mathrm{def}}}}\big(V_{\ell,\rho}(DU(\ell))-V^{\mathrm{hom}}_{,\rho}(DI^{\mathrm{hom}}U(\ell))\big)\cdot D_\rho V(\ell) &(6.96)\\
&\quad+\sum_{\substack{\ell\in\Lambda^{\mathrm{hom}}\\|\ell|\ge r}}\sum_{\substack{\rho\in(\Lambda_*^{\mathrm{hom}}\setminus B_{R_{\mathrm{def}}})-\ell\\|\rho|\ge R_{\mathrm{def}}}}\big(V_{\ell,\rho}(DU(\ell))-V^{\mathrm{hom}}_{,\rho}(DI^{\mathrm{hom}}U(\ell))\big)\cdot D_\rho V(\ell) &(6.97)\\
&\quad+\sum_{\substack{\ell\in\Lambda^{\mathrm{hom}}\\|\ell|\ge r}}\Bigg(\sum_{\substack{\rho_1\in(\Lambda\cap B_{R_{\mathrm{def}}})-\ell\\|\rho_1|\ge R_{\mathrm{def}}}}V_{\ell,\rho_1}(DU(\ell))\cdot D_{\rho_1}V(\ell)\\
&\qquad\qquad-\sum_{\substack{\rho_2\in(\Lambda_*^{\mathrm{hom}}\cap B_{R_{\mathrm{def}}})-\ell\\|\rho_2|\ge R_{\mathrm{def}}}}V^{\mathrm{hom}}_{,\rho_2}(DI^{\mathrm{hom}}U(\ell))\cdot D_{\rho_2}I^{\mathrm{hom}}V(\ell)\Bigg) &(6.98)\\
&\quad+\sum_{\substack{\ell_1\in\Lambda\\|\ell_1|\le r}}\sum_{\rho_1\in\Lambda-\ell_1}V_{\ell_1,\rho_1}(DU(\ell_1))\cdot D_{\rho_1}V(\ell_1)\\
&\qquad\qquad-\sum_{\substack{\ell_2\in\Lambda^{\mathrm{hom}}\\|\ell_2|\le r}}\sum_{\rho_2\in\Lambda_*^{\mathrm{hom}}}V^{\mathrm{hom}}_{,\rho_2}(DI^{\mathrm{hom}}U(\ell_2))\cdot D_{\rho_2}I^{\mathrm{hom}}V(\ell_2). &(6.99)
\end{aligned}
$$

To estimate (6.96), observe that for $|\ell|\ge r$ that $|\rho|<R_{\mathrm{def}}\le|\ell|-R_{\mathrm{def}}$, hence (6.79) of **(V.H)** and Lemma 6.9 imply

$$
\begin{aligned}
&\Bigg|\sum_{\substack{\ell\in\Lambda^{\mathrm{hom}}\\|\ell|\ge r}}\sum_{\substack{\rho\in\Lambda_*^{\mathrm{hom}}\\|\rho|<R_{\mathrm{def}}}}\big(V_{\ell,\rho}(DU(\ell))-V^{\mathrm{hom}}_{,\rho}(DI^{\mathrm{hom}}U(\ell))\big)\cdot D_\rho V(\ell)\Bigg|\\
&\le C\sum_{\substack{\ell\in\Lambda^{\mathrm{hom}}\\|\ell|\ge r}}\sum_{\substack{\rho\in\Lambda-\ell\\|\rho|<R_{\mathrm{def}}}}e^{-\gamma(|\ell|-R_{\mathrm{def}})}e^{-\gamma|\rho|}|D_\rho V(\ell)|\le C\sum_{\substack{\ell\in\Lambda^{\mathrm{hom}}\\|\ell|\ge r}}e^{-\gamma|\ell|/2}|DV(\ell)|_\gamma\\
&\le C\|e^{-\gamma|\cdot|/2}\|_{\ell^2(\Lambda^{\mathrm{hom}})}\|DV\|_{\ell^2_\gamma(\Lambda^{\mathrm{hom}})}\le C\gamma^{-3/2}\|DV\|_{\ell^2(\Lambda^{\mathrm{hom}})}. &(6.100)
\end{aligned}
$$

An identical argument gives the following estimate for (6.97)

$$
\begin{aligned}
&\Bigg| \sum_{\substack{\ell\in\Lambda^{\rm hom}\\ |\ell|\geq r}} \sum_{\substack{\rho\in(\Lambda_*^{\rm hom}\setminus B_{R_{\rm def}})-\ell\\ |\rho|\geq R_{\rm def}}} \big(V_{\ell,\rho}(DU(\ell)) - V^{\rm hom}_{,\rho}(DI^{\rm hom}U(\ell))\big)\cdot D_\rho V(\ell)\Bigg| \\
&\leq C \sum_{\substack{\ell\in\Lambda^{\rm hom}\\ |\ell|\geq r}} \sum_{\substack{\rho\in\Lambda-\ell\\ |\rho|\geq R_{\rm def}}} e^{-\gamma(|\ell|-R_{\rm def})}e^{-\gamma|\rho|}|D_\rho V(\ell)| \leq C \sum_{\substack{\ell\in\Lambda^{\rm hom}\\ |\ell|\geq r}} e^{-\gamma|\ell|/2}|DV(\ell)|_\gamma \\
&\leq C\|e^{-\gamma|\cdot|/2}\|_{\ell^2(\Lambda^{\rm hom})}\|DV\|_{\ell^2_\gamma(\Lambda^{\rm hom})} \leq C\gamma^{-3/2}\|DV\|_{\ell^2(\Lambda^{\rm hom})}.
\end{aligned}
$$

Consider the following term in (6.98),

$$
\begin{aligned}
&\sum_{\substack{\ell\in\Lambda^{\rm hom}\\ |\ell|\geq r}} \sum_{\substack{\rho\in(\Lambda_*^{\rm hom}\cap B_{R_{\rm def}})-\ell\\ |\rho|\geq R_{\rm def}}} V^{\rm hom}_{,\rho}(DI^{\rm hom}U(\ell))\cdot D_\rho I^{\rm hom}V(\ell) \\
&\qquad\qquad = \sum_{\ell'\in\Lambda^{\rm hom}\cap B_{R_{\rm def}}} \sum_{\substack{\rho'\in(\Lambda^{\rm hom}\setminus B_r)-\ell'\\ |\rho'|\geq R_{\rm def}}} V^{\rm hom}_{,\rho'}(DI^{\rm hom}U(\ell'))\cdot D_{\rho'} I^{\rm hom}V(\ell'),
\end{aligned}
$$

where we have used the substitutions $\ell' = \ell+\rho, \rho' = -\rho$. Applying **(V.L)**, Lemmas 6.9 and 6.10 and Cauchy–Schwarz yields

$$
\begin{aligned}
&\Bigg| \sum_{\ell'\in\Lambda^{\rm hom}\cap B_{R_{\rm def}}} \sum_{\substack{\rho'\in(\Lambda^{\rm hom}\setminus B_r)-\ell'\\ |\rho'|\geq R_{\rm def}}} V^{\rm hom}_{,\rho'}(DI^{\rm hom}U(\ell'))\cdot D_{\rho'} I^{\rm hom}V(\ell')\Bigg| \\
&\leq C \sum_{\ell'\in\Lambda^{\rm hom}\cap B_{R_{\rm def}}} \sum_{\substack{\rho'\in(\Lambda^{\rm hom}\setminus B_r)-\ell'\\ |\rho'|\geq R_{\rm def}}} e^{-\gamma|\rho|}|D_{\rho'} I^{\rm hom}V(\ell')| \\
&\leq C \sum_{\ell'\in\Lambda^{\rm hom}\cap B_{R_{\rm def}}} |DI^{\rm hom}V(\ell')|_\gamma \leq C|\Lambda^{\rm hom}\cap B_{R_{\rm def}}|^{1/2}\|DI^{\rm hom}V\|_{\ell^2_\gamma(\Lambda^{\rm hom})} \\
&\leq C\|DV\|_{\ell^2_\gamma(\Lambda)} \leq C\|DV\|_{\ell^2(\Lambda)}. \qquad (6.101)
\end{aligned}
$$

An identical argument estimates the remaining term in (6.98)

$$
\Bigg| \sum_{\substack{\ell\in\Lambda^{\rm hom}\\ |\ell|\geq r}} \sum_{\substack{\rho\in(\Lambda\cap B_{R_{\rm def}})-\ell\\ |\rho|\geq R_{\rm def}}} V_{\ell,\rho}(DU(\ell))\cdot D_\rho V(\ell)\Bigg| \leq C\|DV\|_{\ell^2(\Lambda)}.
$$

The following term appearing in (6.99) can be estimated as

$$\begin{aligned}
&\Bigg|\sum_{\substack{\ell\in\Lambda^{\mathrm{hom}}\\|\ell|\le r}}\sum_{\rho\in\Lambda_*^{\mathrm{hom}}} V_{,\rho}^{\mathrm{hom}}(DI^{\mathrm{hom}}U(\ell))\cdot D_\rho I^{\mathrm{hom}}V(\ell)\Bigg|\\
&\le C\sum_{\ell\in\Lambda^{\mathrm{hom}}\cap B_r}\sum_{\rho\in\Lambda_*^{\mathrm{hom}}} e^{-\gamma|\rho|}|D_\rho I^{\mathrm{hom}}V(\ell)| \le C\sum_{\ell\in\Lambda^{\mathrm{hom}}\cap B_r}|DI^{\mathrm{hom}}V(\ell)|_\gamma\\
&\le C|\Lambda^{\mathrm{hom}}\cap B_r|^{1/2}\|DI^{\mathrm{hom}}V\|_{\ell^2_\gamma(\Lambda^{\mathrm{hom}})} \le C\|DV\|_{\ell^2(\Lambda)},
\end{aligned}\tag{6.102}$$

and similarly for the remaining term in (6.99)

$$\Bigg|\sum_{\substack{\ell\in\Lambda\\|\ell|\le r}}\sum_{\rho\in\Lambda-\ell} V_{\ell,\rho}(DU(\ell))\cdot D_\rho V(\ell)\Bigg| \le C\|DV\|_{\ell^2(\Lambda)}.\tag{6.103}$$

Collecting the estimates (6.100)–(6.103), we deduce that for $U, V \in \dot{\mathscr{W}}^{\mathrm{c}}(\Lambda)$

$$\left|\sum_{\ell\in\Lambda}\big\langle\delta V_\ell\big(DU(\ell)\big), DV(\ell)\big\rangle - \big\langle\delta\mathscr{E}^{\mathrm{hom}}(U), I^{\mathrm{hom}}V\big\rangle\right| \le C\|DV\|_{\ell^2(\Lambda)},\tag{6.104}$$

then as Theorem 6.15 ensures that $\delta\mathscr{E}^{\mathrm{hom}}(I^{\mathrm{hom}}U)$ is a bounded linear operator on $\dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})$, the series $\sum_{\ell\in\Lambda}\big\langle\delta V_\ell\big(DU(\ell)\big), DV(\ell)\big\rangle$ converges. Repeating the estimate (6.85), it follows that

$$\begin{aligned}
&\left|\mathscr{E}(U+V)-\mathscr{E}(U)-\sum_{\ell\in\Lambda}\big\langle\delta V_\ell\big(DU(\ell)\big), DV(\ell)\big\rangle\right|\\
&\le\left|\sum_{\ell\in\Lambda}\Big(V_\ell(D(U+V)(\ell))-V_\ell(DU(\ell))-\big\langle\delta V_\ell\big(DU(\ell)\big), DV(\ell)\big\rangle\Big)\right|\\
&\le\int_0^1\sum_{\ell\in\Lambda}\big|\big\langle\delta^2 V_\ell\big(D(U+tV)(\ell)\big)DU(\ell), DV(\ell)\big\rangle\big|\ \mathrm{d}t \le C\|DU\|_{\ell^2}\|DV\|_{\ell^2},
\end{aligned}$$

hence for each $U \in \dot{\mathscr{W}}^{\mathrm{c}}(\Lambda)$, $\delta\mathscr{E}(U)$ is a bounded linear functional on $\dot{\mathscr{W}}^{\mathrm{c}}(\Lambda)$ and

$$\langle\delta\mathscr{E}(U), V\rangle = \sum_{\ell\in\Lambda}\big\langle\delta V_\ell\big(DU(\ell)\big), DV(\ell)\big\rangle.\tag{6.105}$$

In particular, this holds for $U \equiv 0$, so $\delta\mathscr{E}(0)$ is a bounded linear functional on $\dot{\mathscr{W}}^{\mathrm{c}}(\Lambda)$. Then, applying Theorem 6.15, it follows that $\mathscr{E}$ can be uniquely extended to $\dot{\mathscr{W}}^{1,2}(\Lambda)$ and is infinitely differentiable. In addition, both (6.104) and (6.105) can be extended to $U, V \in \dot{\mathscr{W}}^{1,2}(\Lambda)$, then combining them yields (6.94)

$$|\langle \delta\mathcal{E}(U), V\rangle - \langle \delta\mathcal{E}^{\mathrm{hom}}(I^{\mathrm{hom}}U), I^{\mathrm{hom}}V\rangle| \leq C\|DV\|_{\ell^2(\Lambda)}.$$

It remains to show (6.95). Other than applying using Lemma 6.11 to estimate

$$\|DI^{\mathrm{def}}V^{\mathrm{hom}}\|_{\ell^2(\Lambda)} \leq \|I^{\mathrm{def}}\|_{\dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}}),\dot{\mathscr{W}}^{1,2}(\Lambda)}\|DV^{\mathrm{hom}}\|_{\ell^2(\Lambda^{\mathrm{hom}})},$$

the proof of (6.94) follows the argument (6.96)–(6.104) verbatim. □

Remark 27. By following the proof of (6.95) in Lemma 6.17 verbatim, we obtain the following estimate by collecting the analogous estimates to (6.101) and (6.102): there exists $C > 0$ and $r' > 0$ such that for all $U \in \dot{\mathscr{W}}^{1,2}(\Lambda, \lambda)$ and $V^{\mathrm{hom}} \in \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})$

$$\begin{aligned}
&\big|\big\langle \delta\mathcal{E}^{\mathrm{hom}}(I^{\mathrm{hom}}\bar{U}), V\big\rangle - \big\langle \delta\mathcal{E}(\bar{U}), I^{\mathrm{def}}V\big\rangle\big| \\
&\quad \leq C\Big(\sum_{\ell\in\Lambda^{\mathrm{hom}}} e^{-\gamma|\ell|/2}|DV^{\mathrm{hom}}(\ell)|_\gamma + \sum_{\ell\in\Lambda^{\mathrm{hom}}\cap B_{r'}} |DV^{\mathrm{hom}}(\ell)|_\gamma\Big) \\
&\qquad + C\sum_{\ell'\in\Lambda\cap B_{r'}} |DI^{\mathrm{def}}V^{\mathrm{hom}}(\ell')|_\gamma.
\end{aligned}$$

Then applying (6.39) of Lemma 6.11, there exists $R \geq r' > 0$ and $\gamma > 0$ such that

$$\begin{aligned}
&\big|\big\langle \delta\mathcal{E}^{\mathrm{hom}}(I^{\mathrm{hom}}\bar{U}), V\big\rangle - \big\langle \delta\mathcal{E}(\bar{U}), I^{\mathrm{def}}V\big\rangle\big| \\
&\quad \leq C\Big(\sum_{\ell\in\Lambda^{\mathrm{hom}}} e^{-\gamma|\ell|/2}|DV^{\mathrm{hom}}(\ell)|_\gamma + \sum_{\ell\in\Lambda^{\mathrm{hom}}\cap B_R} |DV^{\mathrm{hom}}(\ell)|_\gamma\Big) \\
&\quad \leq C\sum_{\ell\in\Lambda^{\mathrm{hom}}} e^{-\gamma|\ell|/2}|DV^{\mathrm{hom}}(\ell)|_\gamma. \qquad (6.106)
\end{aligned}$$

The constants C, γ appearing in (6.106) depend only on λ'. The estimate (6.106) will be used in the proof of Lemma 6.21. □

6.10 Proof of decay of minimisers

In order to show Theorem 6.5, we require the Green's function for the homogeneous lattice Λ^{hom}. The following section is devoted to establishing the Green's function and its decay properties.

6.10.1 Homogeneous difference equation

Let V^{hom} be the homogeneous site potential introduced in Theorem 6.14. We define the homogeneous difference operator $H : \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}}) \to \dot{\mathscr{W}}^{-1,2}(\Lambda^{\mathrm{hom}})$ such that for $U, V \in \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})$

$$\begin{aligned} \big\langle HU, V \big\rangle &:= \sum_{\ell \in \Lambda^{\mathrm{hom}}} \big\langle \delta^2 V^{\mathrm{hom}}(0) DU(\ell), DV(\ell) \big\rangle \\ &= \sum_{\ell \in \Lambda^{\mathrm{hom}}} \sum_{\rho, \varsigma \in \Lambda_*^{\mathrm{hom}}} D_\varsigma U(\ell)^T \cdot V^{\mathrm{hom}}_{,\rho\varsigma}(0) \cdot D_\rho V(\ell). \end{aligned} \tag{6.107}$$

The following result gives an alternate form for the operator H.

Lemma 6.18. *There exists $h : \Lambda^{\mathrm{hom}} \to \mathbb{R}^{3\times 3}$, defined by the convergent series*

$$h(\rho) := -\frac{1}{2} \sum_{\substack{\xi, \tau \in \Lambda_*^{\mathrm{hom}} \\ \xi - \tau = \rho}} V^{\mathrm{hom}}_{,\xi\tau}(0), \tag{6.108}$$

which satisfies

$$\big\langle HU, V \big\rangle = \sum_{\ell \in \Lambda^{\mathrm{hom}}} \sum_{\rho \in \Lambda_*^{\mathrm{hom}}} D_\rho U(\ell)^T \cdot h(\rho) \cdot D_\rho V(\ell). \tag{6.109}$$

Moreover, h satisfies $h(-\rho) = h(\rho)$ for all $\rho \in \Lambda^{\mathrm{hom}}$, $h(0) = -\sum_{\rho \in \Lambda_*^{\mathrm{hom}}} h(\rho)$ and there exist $C, \gamma > 0$ such that

$$|h(\rho)| \le C e^{-\gamma|\rho|/2} \quad \text{for all } \rho \in \Lambda^{\mathrm{hom}}. \tag{6.110}$$

Proof. Expanding and collecting the terms of (6.107) yields

$$\langle HU, V\rangle = \sum_{\ell,m\in\Lambda^{\rm hom}} U(m)^T\Bigg(\sum_{\rho\in\Lambda_*^{\rm hom}} V^{\rm hom}_{,\rho\ (\ell-m+\rho)}(0)\Bigg)V(\ell). \tag{6.111}$$

From (6.108) and using **(SE.I)**, we obtain $h(-\rho)=h(\rho)$ for all $\rho\in\Lambda^{\rm hom}$ and $h(0) = -\sum_{\rho\in\Lambda_*^{\rm hom}} h(\rho)$ from the translation and inversion symmetry of the lattice. Then from (6.109), we deduce

$$\langle HU, V\rangle = \sum_{\ell,m\in\Lambda^{\rm hom}} V(m)^T(-2h(\ell-m))U(\ell), \tag{6.112}$$

then equating (6.111) and (6.112) implies (6.108). To see (6.110), we have from (6.108) and **(V.L)** that

$$\begin{aligned}
|h(\rho)| &\le C\sum_{\xi\in\Lambda_*^{\rm hom}} e^{-\gamma(|\xi|+|\xi+\rho|)} \le C\int_{\mathbb{R}^3} e^{-\gamma(|x|+|x+\rho|)}\,\mathrm{d}x\\
&\le C\int_{\mathbb{R}^3\setminus B(|\rho|/2)} e^{-\gamma(|x|+|x+\rho|)}\,\mathrm{d}x + C\int_{B(|\rho|/2)} e^{-\gamma(|x|+|x+\rho|)}\,\mathrm{d}x \le Ce^{-\gamma|\rho|/2}.
\end{aligned}$$

□

Using $h(-\rho)=h(\rho)$ and $h(0) = -\sum_{\rho\in\Lambda_*^{\rm hom}} h(\rho)$, we have

$$\begin{aligned}
\langle HU, V\rangle &= \sum_{\ell\in\Lambda^{\rm hom}}\sum_{\rho\in\Lambda^{\rm hom}-0} \big(U(\ell+\rho)-U(\ell)\big)^T h(\rho)\big(V(\ell+\rho)-V(\ell)\big)\\
&= -2\sum_{\ell\in\Lambda^{\rm hom}} U(\ell)^T h(0)V(\ell) - 2\sum_{\ell\in\Lambda^{\rm hom}}\sum_{\rho\in\Lambda^{\rm hom}-0} U(\ell-\rho)^T h(\rho)V(\ell)\\
&= -2\sum_{\ell\in\Lambda^{\rm hom}}\sum_{\rho\in\Lambda^{\rm hom}} U(\ell-\rho)^T h(\rho)V(\ell).
\end{aligned} \tag{6.113}$$

Therefore, we have

$$HU = -2h*U := -2\sum_{\rho\in\Lambda^{\rm hom}} U(\ell-\rho)^T h(\rho), \tag{6.114}$$

The following lemma defines a lattice Green's function of the homogeneous difference operator (6.107) and provides estimates for the decay of its derivatives, which are essential for showing the decay of displacements minimising (6.14).

Lemma 6.19. *If* **(LS)** *is satisfied, then*

(i) there exists $\mathcal{G} : \Lambda^{\rm hom} \to \mathbb{R}^{3\times 3}$ such that for any $f : \Lambda^{\rm hom} \to \mathbb{R}^3$ which is compactly supported,

$$H(\mathcal{G} * f) = f;$$

(ii) for $1 \leq j \leq 3$, there exist constants C_j such that

$$|D_{\boldsymbol{\rho}}\mathcal{G}(\ell)| \leq C_j\big(1+|\ell|\big)^{-j-1}\prod_{i=1}^{j}|\rho_i| \qquad \forall\ \boldsymbol{\rho} = (\rho_1,\cdots,\rho_j) \in (\Lambda_*^{\rm hom})^j.$$

The proof of this result follows the proof given in [23, Lemma 6.2] verbatim, hence it is omitted.

With the definition and decay estimates of the lattice Green's function, we are now able to prove decay estimates for the linearised lattice elasticity problem

$$\big\langle HU, V\big\rangle = \big\langle g, DV\big\rangle \qquad \forall\ V \in \dot{\mathscr{W}}^{1,2}(\Lambda^{\rm hom}), \tag{6.115}$$

where $g \in \dot{\mathscr{W}}^{-1,2}\big(\Lambda^{\rm hom}\big)$.

Lemma 6.20. *Let* **(LS)** *be satisfied and $U \in \dot{\mathscr{W}}^{1,2}(\Lambda^{\rm hom})$ solve (6.115) and suppose there exist $C,\gamma > 0$ such that*

$$\big|\big\langle g, DV\big\rangle\big| \leq C\sum_{\ell\in\Lambda^{\rm hom}}\big(e^{-\gamma|\ell|/2} + |DU(\ell)|_\gamma^2\big)\,|DV^{\rm hom}(\ell)|_\gamma. \tag{6.116}$$

Then there exists $C = C(\gamma, \|DU\|_{\ell^2(\Lambda^{\rm hom})}) > 0$ such that for all $\ell \in \Lambda^{\rm hom}$ and $\rho \in \Lambda_*^{\rm hom}$

$$|\rho|^{-1}\big|D_\rho U(\ell)\big| \leq C\big(1+|\ell|\big)^{-3}. \tag{6.117}$$

The following estimate is an immediate consequence of Lemma 6.20, for any $\ell \in \Lambda^{\mathrm{hom}}$ and $\gamma > 0$

$$\big|DU(\ell)\big|_\gamma = \sum_{\rho \in \Lambda_*^{\mathrm{hom}}} e^{-\gamma|\rho|} |D_\rho U(\ell)| \leq C \bigg(\sum_{\rho \in \Lambda_*^{\mathrm{hom}}} |\rho| e^{-\gamma|\rho|} \bigg) (1 + |\ell|)^{-3}$$
$$= C_\gamma (1 + |\ell|)^{-3}.$$

It is possible to extend the statement of Lemma 6.20 to estimate higher derivatives of a minimising displacement, as in [23, Lemma 6.4], however we omit this result for the sake of brevity. This result will be included in [2], which is ongoing work.

Proof of Lemma 6.20. We follow the argument used to show [23, Lemma 6.3]. For $m \in \Lambda^{\mathrm{hom}}$, testing (6.115) with $V(\ell) := D_\sigma \mathcal{G}(\ell - m)$ and $\sigma \in \Lambda_*^{\mathrm{hom}}$ and using Lemma 6.19(i) gives

$$D_\sigma U(m) = \big\langle HU, V \big\rangle = \big\langle g, DV \big\rangle, \tag{6.118}$$

then applying Lemma 6.19(ii) and (6.116), we obtain

$$|D_\sigma U(m)| \leq |\langle g, DV \rangle| \leq C|\sigma| \sum_{\ell \in \Lambda^{\mathrm{hom}}} \left(e^{-\gamma|\ell|/2} + |DU(\ell)|_\gamma^2 \right) \big(1 + |\ell - m|\big)^{-3}. \tag{6.119}$$

Then, using the exponential seminorm (6.30), it follows that

$$\begin{aligned} |DU(m)|_\gamma &= \sum_{\rho \in \Lambda_*^{\mathrm{hom}}} e^{-\gamma|\rho|} |D_\rho U(m)| \\ &\leq C \bigg(\sum_{\rho \in \Lambda_*^{\mathrm{hom}}} |\rho| e^{-\gamma|\rho|} \bigg) \sum_{\ell \in \Lambda^{\mathrm{hom}}} \left(e^{-\gamma|\ell|/2} + |DU(\ell)|_\gamma^2 \right) \big(1 + |\ell - m|\big)^{-3} \\ &\leq C \sum_{\ell \in \Lambda^{\mathrm{hom}}} \left(e^{-\gamma|\ell|/2} + |DU(\ell)|_\gamma^2 \right) \big(1 + |\ell - m|\big)^{-3}. \end{aligned} \tag{6.120}$$

We first estimate the following term in (6.120)

$$
\begin{aligned}
& \sum_{\ell\in\Lambda^{\rm hom}} e^{-\gamma|\ell|/2}\big(1+|\ell-m|\big)^{-3} \\
\le\ & C(1+|m|)^{-3}\sum_{|\ell|\le|m|/2} e^{-\gamma|\ell|/2} + Ce^{-\gamma|m|/4}\sum_{|\ell-m|\le|m|/2}(1+|\ell-m|)^{-3} \\
& +C(1+|m|)^{-3}\sum_{\substack{|\ell|>|m|/2\\ |\ell-m|>|m|/2}}(1+|\ell|)^{-s} \\
\le\ & C\Big((1+|m|)^{-3}+e^{-\gamma|m|/4}\log(2+|m|)\Big) \ \le\ C(1+|m|)^{-3}. \qquad (6.121)
\end{aligned}
$$

It remains to estimate the nonlinear residual term appearing in (6.120). For $r>0$, define $w(r) := \sup_{m\in\Lambda^{\rm hom},\ |m|\ge r}|DU(m)|_\gamma$. Our aim is to show that there exists a constant $C>0$ such that for all $r>0$

$$
w(r)\le C(1+r)^{-3}, \qquad (6.122)
$$

which implies $|DU(\ell)|_\gamma \le C(1+|\ell|)^{-3}$ for all $\ell\in\Lambda^{\rm hom}$. Inserting this into (6.119), we infer

$$
\begin{aligned}
|D_\sigma U(m)| &\le C|\sigma|\sum_{\ell\in\Lambda^{\rm hom}}\big(e^{-\gamma|\ell|/2}+|DU(\ell)|_\gamma^2\big)\big(1+|\ell-m|\big)^{-3} \\
&\le C|\sigma|\sum_{\ell\in\Lambda^{\rm hom}}\big(1+|\ell|\big)^{-6}\big(1+|\ell-m|\big)^{-3}, \qquad (6.123)
\end{aligned}
$$

then repeating the argument (6.120)–(6.121) with (6.123), we obtain the desired estimate (6.117)

$$
|\sigma|^{-1}|D_\sigma U(m)|\le C\Big((1+|m|)^{-3}+(1+|m|)^{-6}\log(2+|m|)\Big)\le C(1+|m|)^{-3}.
$$

In order to show (6.122), consider $|m|\ge 2r$, then applying the triangle inequality and Hölder's inequality, we deduce

$$
\begin{aligned}
&\sum_{\ell\in\Lambda^{\rm hom}} \big(1+|\ell|\big)^{-3}|DU(\ell+m)|_\gamma^2 \\
&\quad= \sum_{|\ell|\geq r} \big(1+|\ell|\big)^{-3}|DU(\ell+m)|_\gamma^2 + \sum_{|\ell|<r} \big(1+|\ell|\big)^{-3}|DU(\ell+m)|_\gamma^2 \\
&\quad\leq (1+r)^{-3}\sum_{|\ell|\geq r} |DU(\ell+m)|_\gamma^2 + w(r)^{3/2}\sum_{|\ell|\leq r} \big(1+|\ell|\big)^{-3}|DU(\ell+m)|_\gamma^{1/2} \\
&\quad\leq C\|DU\|^2_{\ell^2(\Lambda^{\rm hom})}(1+r)^{-3} + w(r)^{3/2}\left\|(1+|\cdot|)^{-3}\right\|_{\ell^{4/3}(\Lambda^{\rm hom})}\|DU\|^{1/2}_{\ell^2(\Lambda^{\rm hom})} \\
&\quad\leq C\left((1+r)^{-3}+w(r)^{3/2}\right). \qquad (6.124)
\end{aligned}
$$

Collecting the estimates (6.120)–(6.121) and (6.124) yields

$$
w(2r) = \sup_{m\in\Lambda^{\rm hom},\ |m|\geq 2r} |DU(m)|_\gamma \leq C(1+r)^{-3} + \eta(r)w(r), \qquad (6.125)
$$

where $\eta(r)=w(r)^{1/2}$ and $\eta(r)\to 0$ as $r\to\infty$, as $DU\in\ell^2(\Lambda^{\rm hom})$. Now, define $v(r):=r^3w(r)$, for $r>0$. Multiplying (6.125) with $(2r)^3$, we obtain

$$
v(2r)\leq C\big(1+\eta(r)v(r)\big). \qquad (6.126)
$$

Since $\eta(r)\to 0$ as $r\to\infty$, there exists $r_0>0$ such that for all $r>r_0$

$$
v(2r)\leq C+\frac{1}{2}v(r) \qquad \forall\ r>r_0. \qquad (6.127)
$$

Arguing by induction as in [23, Lemma 6.3], we infer that v is bounded on $\mathbb{R}_{\geq 0}$, which implies (6.122) holds, completing the proof. □

6.10.2 Proof of Theorem 6.5

We require the following result in order to prove Theorem 6.5.

Lemma 6.21. *Suppose that the conditions of Theorem 6.5 are satisfied, then for any $\bar U\in\dot{\mathscr{W}}^{1,2}(\Lambda,\lambda)$ solving (6.14) there exists $g\in\dot{\mathscr{W}}^{-1,2}(\Lambda^{\rm hom})$ such that*

$$
\big\langle HI^{\rm hom}\bar U, V\big\rangle = \big\langle g, DV\big\rangle \qquad \forall\ V\in\dot{\mathscr{W}}^{1,2}(\Lambda^{\rm hom}),
$$

and there exists $C = C(\lambda'), \gamma = \gamma(\lambda') > 0$ *such that*

$$\left|\left\langle g, DV\right\rangle\right| \le C \sum_{\ell\in\Lambda^{\mathrm{hom}}} \left(e^{-\gamma|\ell|/2} + |DI^{\mathrm{hom}}\bar{U}(\ell)|_\gamma^2\right) |DV^{\mathrm{hom}}(\ell)|_\gamma. \tag{6.128}$$

Proof of Theorem 6.5. By Lemma 6.21 $I^{\mathrm{hom}}\bar{U} \in \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}}, \lambda')$ satisfies the conditions of Lemma 6.20, hence applying Lemma 6.20 gives the desired decay estimate (6.18), using that

$$D_\rho I^{\mathrm{hom}}\bar{U}(\ell) = D_\rho \bar{U}(\ell) \quad \text{for} \quad \ell, \ell+\rho \in \Lambda \setminus B_{R_{\mathrm{def}}}.$$

The remaining estimate (6.17) is then shown by following the proof of [23, Theorem 2.3] verbatim. □

Proof of Lemma 6.21. Consider $\bar{U}$ solving (6.14) and $V^{\mathrm{hom}} \in \dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})$, then let $\tilde{\boldsymbol{V}} = (\tilde{V}_1, \tilde{V}_2, \tilde{V}_3) := (I^{\mathrm{hom}}\bar{U}, I^{\mathrm{hom}}\bar{U}, V^{\mathrm{hom}}) \in \left(\dot{\mathscr{W}}^{1,2}(\Lambda^{\mathrm{hom}})\right)^3$. Using that $\delta\mathcal{E}^{\mathrm{hom}}(0) = \delta\mathcal{E}(\bar{U}) = 0$, we rewrite the residual $\left\langle HI^{\mathrm{hom}}\bar{U}, V^{\mathrm{hom}}\right\rangle$ as

$$\begin{aligned}
\left\langle HI^{\mathrm{hom}}\bar{U}, V^{\mathrm{hom}}\right\rangle &= \left\langle \delta^2\mathcal{E}^{\mathrm{hom}}(0) I^{\mathrm{hom}}\bar{U}, V^{\mathrm{hom}}\right\rangle \\
&= \left\langle \delta\mathcal{E}^{\mathrm{hom}}(0) + \delta^2\mathcal{E}^{\mathrm{hom}}(0)I^{\mathrm{hom}}\bar{U} - \delta\mathcal{E}^{\mathrm{hom}}(I^{\mathrm{hom}}\bar{U}), V^{\mathrm{hom}}\right\rangle \qquad (6.129)\\
&\quad + \left\langle \delta\mathcal{E}^{\mathrm{hom}}(I^{\mathrm{hom}}\bar{U}), V^{\mathrm{hom}}\right\rangle - \left\langle \delta\mathcal{E}(\bar{U}), I^{\mathrm{def}}V^{\mathrm{hom}}\right\rangle. \qquad (6.130)
\end{aligned}$$

We estimate (6.129) using the estimate (6.86) from the proof of Theorem 6.15,

$$\begin{aligned}
&\left|\left\langle \delta\mathcal{E}^{\mathrm{hom}}(0) + \delta^2\mathcal{E}^{\mathrm{hom}}(0)I^{\mathrm{hom}}\bar{U} - \delta\mathcal{E}^{\mathrm{hom}}(I^{\mathrm{hom}}\bar{U}), V^{\mathrm{hom}}\right\rangle\right| \\
&\quad \le \int_0^1 (1-t) \left|\left\langle \delta^3\mathcal{E}^{\mathrm{hom}}(tI^{\mathrm{hom}}\bar{U}), \tilde{\boldsymbol{V}}\right\rangle\right| \,\mathrm{d}t \le C \sum_{\ell\in\Lambda} \prod_{m=1}^{3} |D\tilde{V}_m(\ell)|_\gamma \\
&\quad = C \sum_{\ell\in\Lambda} |DI^{\mathrm{hom}}\bar{U}(\ell)|_\gamma^2 |DV^{\mathrm{hom}}(\ell)|_\gamma. \qquad (6.131)
\end{aligned}$$

We estimate (6.130) using the estimate (6.106) shown in Remark 27

$$\left|\left\langle \delta\mathcal{E}^{\mathrm{hom}}(I^{\mathrm{hom}}\bar{U}), V^{\mathrm{hom}}\right\rangle - \left\langle \delta\mathcal{E}(\bar{U}), I^{\mathrm{def}}V^{\mathrm{hom}}\right\rangle\right| \le C \sum_{\ell\in\Lambda^{\mathrm{hom}}} e^{-\gamma|\ell|/2} |DV^{\mathrm{hom}}(\ell)|_\gamma. \tag{6.132}$$

Combining the estimates (6.131)–(6.132) gives the desired result (6.128). □

Chapter 7

Conclusion

We finish by summarising the main results of the thesis and discussing related open problems.

In Chapter 2, we establish uniform regularity estimates for the solution of the TFW equations, corresponding to a nuclear configuration m belonging to spaces such as $\mathcal{M}_{L^2}(M,\omega)$ or $\mathcal{M}_{H^k}(M,\omega)$, for $k \in \mathbb{N}$. This guarantees that $m \in L^2_{\mathrm{unif}}(\mathbb{R}^3)$, which allows for a smeared nuclei description but excludes point nuclei. We believe that by adapting the arguments presented in [16, Propositions 3.8, 3.10, 3.12], it possible to obtain weaker uniform regularity estimates for the TFW ground states corresponding to nuclei configurations defined by a non-negative measure m, satisfying

$$\sup_{x \in \mathbb{R}^3} m(x + B_1) \leq M, \qquad \inf_{x \in \mathbb{R}^3} m(x + B_R) \geq \omega_0 R^3 - \omega_1,$$

for all $R > 0$, where $\omega_0 > 0$ and $\omega_1 \geq 0$.

In Chapter 3, we apply our uniform regularity estimates to prove locality estimates for the TFW equations by adapting the uniqueness proof for the TFW equations in [16]. One can not directly extend our locality results to the point nuclei setting as our proofs make full use of the regularity afforded by the smeared nuclear description. However, it may be possible to adapt the uniqueness proof of the TFW equations for point nuclei [16, Lemma 5.5] to establish weaker locality results for the TFW model in the point nuclei setting, though we expect this to be nontrivial.

In Chapter 4, we collect further applications of our locality results.

One application that we have omitted involves studying the Fermi level associated with the TFW equations [14, 16]. The Fermi level is the Lagrange multiplier appearing in the TFW equations due to the charge neutrality constraint present in the variational problem (1.2), which we now recall. For $m \in \mathcal{M}_{L^2}(M, \omega)$ and $R > 0$, let $m_R = m \cdot \chi_{B_R(0)}$ and consider

$$I^{\mathrm{TFW}}(m_R) = \inf \left\{ E^{\mathrm{TFW}}(v, m_R) \,\middle|\, v \in H^1(\mathbb{R}^3), v \geq 0, \int_{\mathbb{R}^3} v^2 = \int_{\mathbb{R}^3} m_R \right\}.$$

It was established earlier that there exists a unique minimiser u_R, which solves the Euler–Lagrange equation

$$-\Delta u_R + \frac{5}{3} u_R^{7/3} - (m_R - u_R^2) u_R = -\theta_R u_R,$$

where $\theta_R \in \mathbb{R}$ is the Fermi level. Moreover, it is established in [16, Proposition 3.4], that there exists $C > 0$ such that $0 < \theta_R \leq C$ for all $R > 0$. Consequently, passing to the limit as $R \to \infty$, along a subsequence $\theta_R \to \theta$, so we can define a Fermi level θ for the TFW model corresponding to the nuclear configuration m, though it remains to verify whether it is a uniquely defined quantity.

Supposing for now that the Fermi level is unique, one could pursue the following problem: given two nuclear configurations $m_1, m_2 \in \mathcal{M}_{L^2}(M, \omega)$ with corresponding Fermi levels θ_1, θ_2, can one prove that $\theta_1 = \theta_2$ provided that $m_1 - m_2$ decays sufficiently fast?

This question is closely related to an argument used in [18], which freezes the Fermi level in order to obtain locality estimates for the tight binding model. We remark that we have applied similar reasoning in order to show locality estimates for the TFW Yukawa model. For finite systems, the TFW Yukawa variational problem (2.81) does not include a charge neutrality constraint, hence no Lagrange multiplier appears in the TFW Yukawa equations. Adding a charge neutrality constraint to (2.81) introduces a Fermi level that significantly weakens the Yukawa locality results presented in Section 3.1.2.

In Chapter 5, we show the existence, uniqueness and locality results for all variations of the TFW equations and use this to construct site energies with exponentially decaying interaction. We then apply these results in Chapter 6 to consider the TFW lattice relaxation problem for point defects. This introduces a variational problem over a space of nuclear arrangements, which we show is well-defined and also establish decay properties for minimising arrangements, up to first order. Our results could be improved by showing the higher order regularity of the energy difference functional and subsequently obtaining higher order decay estimates for minimising arrangements. We expect this to be a relatively straightforward application of the results shown in Chapter 5 and the analysis performed in [23].

As [23] also considers the relaxation of a crystal due to a straight line dislocation, we believe it is possible to treat dislocations using the TFW model. Additionally, the main application of the decay results established in [23] is to obtain rigorous error estimates for numerical simulations of the lattice relaxation problem. This involves approximating the full, infinite problem with a problem over a finite domain and employing suitable boundary conditions. We intend to apply this idea to the TFW model, and impose boundary conditions on both the electron density and the nuclear charge density. This introduces a PDE problem on a finite domain, which would allow for numerical simulations of the TFW relaxation problem.

One final application of our work is to extend the Coulomb and Yukawa site energy comparison result Theorem 5.2 to higher orders. Though we have focused on studying the TFW lattice relaxation problem using the Coulomb interaction, the entire analysis also holds with the Yukawa interaction. By generalising Theorem 5.2 to higher orders, we believe that it is possible to show the convergence of minimisers of the Yukawa relaxation problem to the Coulomb problem and also estimate the convergence rate. We intend to explore this problem in future work.

In this thesis we have explored the locality of the TFW model and its applications. The broader question of whether other DFT models possess locality properties, and whether this can be proved mathematically is largely open. In future work, we intend to study the locality of the reduced Hartree–Fock Yukawa model [1] as well as generalising the lattice relaxation problem to general models with well-behaved site energies [2]. This work will address some of the open problems mentioned earlier. This includes showing higher order decay for minimisers of the TFW relaxation problem as well as treating the TFW dislocation case.

Appendix A

Proof of Proposition 2.15

This appendix contains the proof of the Yukawa uniqueness result Proposition 2.15.

Proposition 2.15. *Let $a_0 > a_c > 0$ and $m \in \mathcal{M}_{L^2}(M, \omega)$, then for all $0 < a \leq a_0$ the corresponding Yukawa ground state $(u_a, \phi_a) \in H^4_{\mathrm{unif}}(\mathbb{R}^3) \times H^2_{\mathrm{unif}}(\mathbb{R}^3)$ is unique and there exists $c_{a_0,M,\omega} > 0$ such that the electron density u_a satisfies*

$$\inf_{x \in \mathbb{R}^3} u_a(x) \geq c_{a_0,M,\omega} > 0. \tag{2.80}$$

We show Proposition 2.15 by adapting the argument described in [16, Remark 4.16, Lemma 4.14], which shows that the periodic Yukawa ground state is bounded below and hence unique. The proof requires the following result.

Lemma A.1. *For any $a_0 > 0$ and $m \in \mathcal{M}_{L^2}(M, \omega)$, there exists $R_0 = R_0(a_0, \omega)$, $\nu_{a_0,M,\omega} > 0$ such that for all $0 < a \leq a_0$ and $R_n \geq R_0$*

$$\inf_{x \in B_1(0)} u_{a,R_n}(x) \geq \nu_{a_0,M,\omega} > 0. \tag{A.1}$$

Then, sending $R_n \to \infty$ in (A.1), it follows that for all $0 < a \leq a_0$

$$\inf_{x \in B_1(0)} u_a(x) \geq \nu_{a_0,M,\omega} > 0,$$

hence $u_a > 0$. Then following the proof of [16, Lemma 4.14] gives the desired estimate (2.113). As the argument used in [16, Lemma 4.14] is also necessary to show Lemma A.1, it is followed closely in this instance and for the proof of Proposition 2.15, only the necessary changes in the argument are described. In order to prove Lemma A.1, we require the following result.

Lemma A.2. *There exist $R_0' = R_0'(M,\omega) > 0$ and $\nu_{a_{\mathrm{c},\mathrm{M},\omega}} > 0$ such that for all $m \in \mathcal{M}_{L^2}(M,\omega), 0 < a \le a_\mathrm{c}$ and $R_n \ge R_0'$*

$$\inf_{x\in B_1(0)} u_{a,R_n}(x) \ge \nu_{a_\mathrm{c},M,\omega} > 0. \tag{A.2}$$

Proof of Lemma A.2. We show (A.2) by contradiction, so suppose that for all $R_0' > 0$

$$\inf_{0<a\le a_\mathrm{c}} \inf_{R_n \ge R_0'} \inf_{m\in\mathcal{M}_{L^2}(M,\omega)} \inf_{x\in B_1(0)} u_{a,R_n,m}(x) = 0,$$

where $u_{a,R_n,m}$ solves (2.3a) corresponding to $m_{R_n} = m\cdot\chi_{B_{R_n}(0)}$. Hence for each $k\in\mathbb{N}$ there exist sequences $(a_k) \subset (0,a_\mathrm{c}]$ converging to some $a_* \in [0,a_\mathrm{c}]$, $R_{n_k} \uparrow \infty$, $\widetilde{m}_k \in \mathcal{M}_{L^2}(M,\omega)$ and $x_k \in B_1(0)$ such that $m_{k,R_{n_k}} = \widetilde{m}_k \cdot \chi_{B_{R_{n_k}}(0)}$ satisfies for all $k\in\mathbb{N}$

$$u_{a_k,R_{n_k},\widetilde{m}_k}(x_k) \le \frac{1}{k}.$$

For convenience, in this argument $u_{a_k,R_{n_k},\widetilde{m}_k}$ and $m_{k,R_{n_k}}$ are referred to as u_k and m_k, respectively. By the Harnack inequality [28, Theorem 8.20], for fixed $k\in\mathbb{N}$ and any $R'\ge 1$ there exists $C(R',a_0,M) > 0$ such that

$$\sup_{x\in B_{R'}(0)} u_k(x) \le C \inf_{x\in B_{R'}(0)} u_k(x) \le \frac{C(R',a_0,M)}{k}, \tag{A.3}$$

so it follows that u_k converges uniformly to 0 on any compact subset as $k\to\infty$. Let (u_k,ϕ_k) denote the solution of (2.3) corresponding to m_k with screening parameter a_k. Recall that ϕ_k solves the following equation in the sense of distributions

$$-\Delta\phi_k + a_k^2\,\phi_k = 4\pi\left(m_k - u_k^2\right). \tag{A.4}$$

We pass to the limit in (A.4) as $k \to \infty$, using the following estimates

$$\|m_k\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq M,$$
$$\|\phi_k\|_{H^2_{\mathrm{unif}}(\mathbb{R}^3)} \leq C(M).$$

It follows that, up to a subsequence, ϕ_k converges to $\widetilde{\phi}$, weakly in $H^2(B_R(0))$, strongly in $H^1(B_R(0))$ for all $R > 0$ and pointwise almost everywhere. Moreover, m_k converges to $\widetilde{m}$, weakly in $L^2(B_R(0))$ for all $R > 0$. Applying the estimates (2.64)–(2.65) verbatim, it follows that $\widetilde{m} \in \mathcal{M}_{L^2}(M, \omega)$. Passing to the limit in (A.4) and using that $a_k \to a_* \in [0, a_{\mathrm{c}}]$ it follows that $\widetilde{\phi}$ is a distributional solution of

$$-\Delta\widetilde{\phi} + a_*^2\,\widetilde{\phi} = 4\pi\widetilde{m}. \tag{A.5}$$

We now show that (2.116) leads to a contradiction. If $a_* = 0$, then observe that (A.5) becomes (2.66) from Proposition 2.2. Applying the argument in Proposition 2.2 verbatim leads to the contradiction that $\widetilde{m} \notin \mathcal{M}_{L^2}(M, \omega)$.

Alternatively, suppose $a_* \in (0, a_{\mathrm{c}}]$ and define $\widetilde{u} \equiv 0$. It follows immediately that $(\widetilde{u}, \widetilde{\phi})$ solves (2.3) corresponding to $\widetilde{m}$ with screening parameter a_*. As $a_* \in (0, a_{\mathrm{c}}]$, Proposition 2.14 applies, hence $(\widetilde{u}, \widetilde{\phi})$ is the unique Yukawa ground state corresponding to $\widetilde{m}$ and $\widetilde{u}$ satisfies $\inf \widetilde{u} \geq c_{a_{\mathrm{c}},\mathrm{M},\omega} > 0$, which contradicts that $\widetilde{u} \equiv 0$. Consequently, the desired estimate (A.2) holds. □

Proof of Lemma A.1. As Lemma A.2 shows that there exists $R_0' > 0$ such that for all $0 < a \leq a_{\mathrm{c}}$

$$\inf_{R_n \geq R_0'} \inf_{m \in \mathcal{M}_{L^2}(M,\omega)} \inf_{x \in B_1(0)} u_{a,R_n,m}(x) \geq \nu_{a_{\mathrm{c}},M,\omega} > 0,$$

it remains to show that there exists $R_0 > 0$ such that for all $a_{\mathrm{c}} < a \leq a_0$

$$\inf_{R_n \geq R_0} \inf_{m \in \mathcal{M}_{L^2}(M,\omega)} \inf_{x \in B_1(0)} u_{a,R_n,m}(x) \geq \nu'_{a_0,M,\omega} > 0. \tag{A.6}$$

The estimate (A.6) is shown by contradiction, so suppose that for all $R_0 > 0$

$$\inf_{a_{\mathrm{c}} < a \leq a_0} \inf_{R_n \geq R_0} \inf_{m \in \mathcal{M}_{L^2}(M,\omega)} \inf_{x \in B_1(0)} u_{a,R_n,m}(x) = 0, \tag{A.7}$$

where $u_{a,R_n,m}$ solves (2.3a) corresponding to $m_{R_n} = m \cdot \chi_{B_{R_n}(0)}$. Hence for each $k \in \mathbb{N}$ there exist sequences $(a_k) \subset (a_c, a_0]$, $R_{n_k} \uparrow \infty$, $\widetilde{m}_k \in \mathcal{M}_{L^2}(M, \omega)$ and $x_k \in B_1(0)$ such that $m_{k,R_{n_k}} = \widetilde{m}_k \cdot \chi_{B_{R_{n_k}}(0)}$ satisfies for all $k \in \mathbb{N}$

$$u_{a_k,R_{n_k},\widetilde{m}_k}(x_k) \leq \frac{1}{k}.$$

For convenience, in this argument $u_{a_k,R_{n_k},\widetilde{m}_k}$ and $m_{k,R_{n_k}}$ are referred to as u_k and m_k, respectively. Applying the argument used to show (2.115) verbatim, the Harnack inequality implies that for every $R' \geq 1$ there exists $C(R', a_0, M) > 0$ such that for all $k \in \mathbb{N}$

$$\sup_{x \in B_{R'}(0)} u_k(x) \leq C \inf_{x \in B_{R'}(0)} u_k(x) \leq \frac{C(R', a_0, M)}{k}, \tag{A.8}$$

so it follows that u_k converges uniformly to 0 on any compact subset as $k \to \infty$. For $R > 0$ and $k \in \mathbb{N}$, define the energy functional acting on v satisfying $\nabla v \in L^2(B_R(0))$ and $v \in L^{10/3}(B_R(0))$ by

$$\begin{aligned} E(v; k, R) = &\int_{B_R(0)} |\nabla v|^2 + \int_{B_R(0)} v^{10/3} - \int_{B_R(0)} (m_k * Y_{a_k}) v^2 \\ &+ \frac{1}{2} \int_{B_R(0)} \left(v^2 \cdot \chi_{B_R(0)} * Y_{a_k}\right) v^2 + \int_{B_R(0)} \left(u_k^2 \cdot \chi_{B_R(0)^c} * Y_{a_k}\right) v^2. \end{aligned}$$

Then consider the corresponding variational problem

$$I(k, R) = \inf \left\{ E(v; k, R) \,\middle|\, \nabla v \in L^2(B_R(0)), v \in L^{10/3}(B_R(0)), v|_{\partial B_R(0)} = u_k \right\}. \tag{A.9}$$

The construction of the energy and the boundary condition of (A.9) ensures that u_k is the unique minimiser of (A.9) for each $R > 0$. To prove this, observe that $E(v; k, R)$ can be expressed as

$$\begin{aligned} E(v; k, R) = &\int_{B_R(0)} |\nabla v|^2 + \int_{B_R(0)} v^{10/3} + \int_{B_R(0)} \left(u_k^2 \cdot \chi_{B_R(0)^c} * Y_{a_k}\right) v^2 \\ &+ \frac{1}{2} D_{a_k}\left(m_k - v^2 \chi_{B_R(0)}, m_k - v^2 \chi_{B_R(0)}\right) - \frac{1}{2} D_{a_k}(m_k, m_k). \end{aligned}$$

As Y_{a_k} and the Yukawa interaction term are non-negative, it follows that

$$\begin{aligned} E(v;k,R) &\geq \int_{B_R(0)} |\nabla v|^2 + \int_{B_R(0)} v^{10/3} - \frac{1}{2} D_{a_k}(m_k, m_k) \\ &\geq -\frac{1}{2} D_{a_k}(m_k, m_k) > -\infty, \end{aligned}$$

so as $E(v;k,R)$ is bounded below, $I(k,R)$ is well-defined. Any minimising sequence v_n satisfies

$$\|\nabla v_n\|_{L^2(B_R(0))}^2 + \|v_n\|_{L^{10/3}(B_R(0))}^{10/3} \leq C(k,R,a_0,M),$$

hence there exists $v_{k,R}$ such that $\nabla v_{k,R} \in L^2(\mathbb{R}^3), v_{k,R} \in L^{10/3}(\mathbb{R}^3)$. Moreover, along a subsequence ∇v_n converges to $\nabla v_{k,R}$ weakly in $L^2(\mathbb{R}^3)$, v_n converges to $v_{k,R}$, weakly in $L^6(\mathbb{R}^3)$ and $L^{10/3}(\mathbb{R}^3)$, strongly in $L^p(B_R(0))$ for all $p \in [1,6)$ and $R > 0$ and pointwise almost everywhere. Moreover, $v_{k,R}$ satisfies

$$E(v_{k,R};k,R) = I(k,R),$$

and solves

$$\begin{aligned} -\Delta v_{k,R} + \frac{5}{3} v_{k,R}^{7/3} + \left(m_k - v_{k,R}^2 \cdot \chi_{B_R(0)} - u_k^2 \cdot \chi_{B_R(0)^c}\right) v_{k,R} = 0, \quad \text{(A.10)} \\ v_{k,R} = u_k \quad \text{on } \partial B_R(0). \end{aligned}$$

It is straightforward to verify that u_k solves (A.10). Define the alternate minimisation problem

$$\inf \left\{ E(\sqrt{\rho};k,R) \,\middle|\, \nabla\sqrt{\rho} \in L^2(\mathbb{R}^3), \rho \in L^{5/3}(\mathbb{R}^3), \rho \geq 0 \right\}. \qquad \text{(A.11)}$$

Due to the strict convexity of $\rho \mapsto E(\sqrt{\rho};k,R)$, it follows that $\rho_k = u_k^2$ is the unique minimiser of (A.11), hence u_k is the unique minimiser of (A.9).

As $u_k \to 0$ uniformly as $k \to \infty$, it follows that for any fixed $R > 0$

$$E(u_k;k,R) \to 0 \quad \text{as} \quad k \to \infty. \qquad \text{(A.12)}$$

To verify (A.12), observe that

$$
\begin{aligned}
E(u_k; k, R) = &\int_{B_R(0)} |\nabla u_k|^2 + \int_{B_R(0)} u_k^{10/3} - \int_{B_R(0)} \left(m_k * Y_{a_k}\right) u_k^2 \\
&+ \frac{1}{2}\int_{B_R(0)} \left(u_k^2 \cdot \chi_{B_R(0)} * Y_{a_k}\right) u_k^2 + \int_{B_R(0)} \left(u_k^2 \cdot \chi_{B_R(0)^c} * Y_{a_k}\right) u_k^2.
\end{aligned}
$$

Clearly

$$
0 \leq \int_{B_R(0)} u_k^{10/3} \leq CR^3 \|u_k\|_{L^\infty(B_R(0))}^{10/3} \to 0 \text{ as } k \to \infty. \tag{A.13}
$$

The term $m_k * Y_{a_k}$ can be estimated by

$$
\|m_k * Y_{a_k}\|_{L^\infty(\mathbb{R}^3)} \leq C(a_{\mathrm{c}}, M), \tag{A.14}
$$

where the constant $C(a_{\mathrm{c}}, M)$ is independent of $k \in \mathbb{N}$. From (A.14) it follows that

$$
\begin{aligned}
\left| \int_{B_R(0)} \left(m_{k,j} * Y_{a_k}\right) u_k^2 \right| &\leq \|m_k * Y_{a_k}\|_{L^\infty(\mathbb{R}^3)} \int_{B_R(0)} u_k^2 \\
&\leq C a_{\mathrm{c}}^{-3} M R^3 \|u_k\|_{L^\infty(B_R(0))}^2 \to 0 \text{ as } k \to \infty.
\end{aligned}
$$

To show (A.14), let $\Gamma \subset \mathbb{R}^3$ be a semi-open unit cube centred at the origin, so $\mathbb{R}^3 = \{\, \Gamma + i \,|\, i \in \mathbb{Z}^3 \,\}$. For any $x \in \mathbb{R}^3$

$$
\begin{aligned}
\left|\left(m_k * Y_{a_k}\right)(x)\right| &\leq \int_{\mathbb{R}^3} |m_k(x-y)| \frac{e^{-a_k|y|}}{|y|} \,\mathrm{d}y = \sum_{i \in \mathbb{Z}^3} \int_{\Gamma+i} |m_k(x-y)| \frac{e^{-a_k|y|}}{|y|} \,\mathrm{d}y \\
&\leq C \sum_{i \in \mathbb{Z}^3} \|m_k\|_{L^2_{\mathrm{unif}}(\mathbb{R}^3)} \left\| \tfrac{e^{-a_k|\cdot|}}{|\cdot|} \right\|_{L^2(\Gamma+i)} \leq CM \sum_{i \in \mathbb{Z}^3} \left\| \tfrac{e^{-a_k|\cdot|}}{|\cdot|} \right\|_{L^2(\Gamma+i)} \\
&\leq CM \sum_{i \in \mathbb{Z}^3} e^{-a_k|i|} \leq \frac{CM}{a_k^3} \leq \frac{CM}{a_{\mathrm{c}}^3}.
\end{aligned} \tag{A.15}
$$

As the estimate (A.15) is independent of $k \in \mathbb{N}$ and $x \in \mathbb{R}^3$, (A.14) holds.

Estimating the remaining terms gives

$$\begin{aligned}\frac{1}{2}\int_{B_R(0)}\left(u_k^2\cdot\chi_{B_R(0)} * Y_{a_k}\right)u_k^2 &\le \|u_k\|^4_{L^\infty(B_R(0))}D_{a_k}(\chi_{B_R(0)},\chi_{B_R(0)})\\ &\le Ca_{\mathrm{c}}^{-2}R^3\|u_k\|^4_{L^\infty(B_R(0))}\to 0 \text{ as } k\to\infty,\end{aligned}$$

$$\begin{aligned}\int_{B_R(0)}\left(u_k^2\cdot\chi_{B_R(0)^c} * Y_{a_k}\right)u_k^2 &\le \left\|u_k^2\cdot\chi_{B_R(0)^c} * Y_{a_k}\right\|_{L^\infty(\mathbb{R}^3)}\int_{B_R(0)}u_k^2\\ &\le CR^3\|u_k\|^2_{L^\infty(\mathbb{R}^3)}\left\|Y_{a_k}\right\|_{L^1(\mathbb{R}^3)}\|u_k\|^2_{L^\infty(B_R(0))}\\ &\le \frac{C(a_0,M)R^3}{a_{\mathrm{c}}^2}\|u_k\|^2_{L^\infty(B_R(0))}\to 0 \text{ as } k\to\infty.\end{aligned}$$

For the final term, integration by parts yields

$$\begin{aligned}\int_{B_R(0)}|\nabla u_k|^2 &= -\int_{B_R(0)}u_k\,\Delta u_k + \int_{\partial B_R(0)}u_k\frac{\partial u_k}{\partial n}\\ &\le C\|u_k\|_{W^{2,\infty}(\mathbb{R}^3)}(R^3+R^2)\|u_k\|_{L^\infty\left(\overline{B_R(0)}\right)}\\ &\le C(a_0,M)R^3\|u_k\|_{L^\infty(B_R(0))}\to 0 \text{ as } k\to\infty.\end{aligned}\tag{A.16}$$

Collecting (A.13)–(A.16), it follows that for fixed $R>0$, $E(u_k;k,R)\to 0$ as $k\to\infty$. A family of test functions $\varphi_{\varepsilon,k}\in H^1(B_R(0))$ is now constructed, satisfying the boundary condition $\varphi_{\varepsilon,k}|_{\partial B_R(0)}=u_k$ of (A.9) such that for sufficiently large $R>0$ and small $\varepsilon>0$, there exists a constant $C_1>0$ such that for all large $k\in\mathbb{N}$

$$E(\varphi_{\varepsilon,k};k,R)\le -C_1<0,\tag{A.17}$$

contradicting the fact that $E(u_k;k,R)\to 0$ as $k\to\infty$, as (A.17) implies

$$E(u_k;k,R)\le E(\varphi_{\varepsilon,k};k,R)\le -C_1<0.$$

Lemma 2.10 will be used to prove (A.17) by showing that there exists $R_0'\ge R_0$

and $k_1 \in \mathbb{N}$ such that choosing $R_n = R_0'$ and $k \geq k_1$ ensures

$$\int_{B_{4R_0'}(0)} |\nabla \psi_{R_0'}|^2 + \int_{B_{4R_0'}(0)} \left(\left(u_k^2 \cdot \chi_{B_{4R_0'}(0)^c} - m_k\right) * Y_{a_k}\right) \psi_{R_0'}^2 \leq -1. \tag{A.18}$$

Recall Lemma 2.10, that there exists $C_0 = C_0(a_c, a_0, \omega) > 0$ and $R_0 = R_0(a_c, a_0, \omega) > 0$ such that for any $a_c < a \leq a_0$ and $R_n \geq R_0$

$$\int_{\mathbb{R}^3} |\nabla \psi_{R_n}|^2 - D_a(m_{R_n}, \psi_{R_n}^2) \leq -C_0 R_n^3, \tag{A.19}$$

The following term can be estimated and decomposed as

$$\begin{aligned} \int_{B_{4R_n}(0)} \left(\left(u_k^2 \cdot \chi_{B_{4R_n}(0)^c}\right) * Y_{a_k}\right) \psi_{R_n}^2 &\leq \int_{B_{4R_n}(0)} \left(\left(u_k^2 \cdot \chi_{B_{4R_n}(0)^c}\right) * Y_{a_k}\right) \\ = \int_{B_{4R_n}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_n}(0)^c}\right) * Y_{a_k}\right) &+ \int_{B_{4R_n}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_n}(0) \setminus B_{4R_n}(0)}\right) * Y_{a_k}\right). \end{aligned} \tag{A.20}$$

The first term of (A.20) can be expressed as

$$\int_{B_{4R_n}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_n}(0)^c}\right) * Y_{a_k}\right) = \int_{B_{8R_n}(0)^c} u_k^2(y) \left(\int_{B_{4R_n}(0)} \frac{e^{-a_k|x-y|}}{|x-y|} \, \mathrm{d}x\right) \mathrm{d}y.$$

By the triangle inequality $|x-y| \geq \frac{|y|}{2}$, hence

$$\begin{aligned} &\int_{B_{4R_n}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_n}(0)^c}\right) * Y_{a_k}\right) \\ &\qquad \leq \|u_k\|_{L^\infty(\mathbb{R}^3)}^2 \int_{B_{8R_n}(0)^c} \left(\int_{B_{4R_n}(0)} \frac{e^{-a_c|y|/2}}{|y|} \, \mathrm{d}x\right) \mathrm{d}y \\ &\qquad = C R_n^3 \int_{B_{8R_n}(0)^c} \frac{e^{-a_c|y|/2}}{|y|} \, \mathrm{d}y = C a_c^{-2} R_n^3 \left(1 + 4 a_c R_n\right) e^{-4 a_c R_n} \\ &\qquad \leq C a_c^{-2} R_n^3 e^{-2 a_c R_n}. \end{aligned}$$

As $e^{-2a_c R_n} \to 0$ as $R_n \to \infty$, there exists $R_2 > 0$ such that for $R_n \geq R_2$

$$\int_{B_{4R_n}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_n}(0)^c}\right) * Y_{a_k}\right) \leq C a_c^{-2} R_n^3 e^{-2a_c R_n} \leq \frac{C_0}{4} R_n^3.$$

Now define $R_0' = \max\{R_0, R_2, (2C_0)^{-1/3}\}$ and choose $R_n = R_0'$. The second term of (A.20) can be estimated using Young's inequality for convolutions

$$
\begin{aligned}
\int_{B_{4R_0'}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_0'}(0)\setminus B_{4R_0'}(0)}\right) * Y_{a_k}\right) &\leq \int_{B_{4R_0'}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_0'}(0)}\right) * Y_{a_k}\right) \\
&\leq CR_0'^3 \|Y_{a_k}\|_{L^1(\mathbb{R}^3)} \|u_k\|^2_{L^\infty(B_{8R_0'}(0))} \leq Ca_{\mathrm{c}}^{-2} R_0'^3 \|u_k\|^2_{L^\infty(B_{8R_0'}(0))}.
\end{aligned}
$$

As $u_k \to 0$ on compact sets, there exists $k_1 \in \mathbb{N}$ such that $k \geq k_1$ ensures that

$$
\int_{B_{4R_0'}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_0'}(0)\setminus B_{4R_0'}(0)}\right) * Y_{a_k}\right) \leq Ca_{\mathrm{c}}^{-2} R_0'^3 \|u_k\|^2_{L^\infty(B_{8R_0'}(0))} \leq \frac{C_0}{4} R_0'^3. \tag{A.21}
$$

Choose $R_n = R_0'$ and recall that $R_{n_k} \uparrow \infty$, hence there exists $k_2 \in \mathbb{N}$ such that $R_{n_k} \geq R_0'$ for all $k \geq k_2$, so it follows that $m_k \geq m_{R_n}$. Collecting the estimates (A.19), (A.20)–(A.21) with $R_n = R_0'$ and observing that $\frac{C_0}{4} R_0'^3 \geq 1$ yields the desired estimate (A.18)

$$
\begin{aligned}
&\int_{B_{4R_0'}(0)} |\nabla \psi_{R_0'}|^2 + \int_{B_{4R_0'}(0)} \left(\left(u_k^2 \cdot \chi_{B_{4R_0'}(0)^c} - m_k\right) * Y_{a_k}\right) \psi_{R_0'}^2 \\
&\qquad \leq \int_{\mathbb{R}^3} |\nabla \psi_{R_0'}|^2 - D_a(m_{R_0'}, \psi_{R_0'}^2) + \int_{B_{4R_0'}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_0'}(0)^c}\right) * Y_{a_k}\right) \\
&\qquad\qquad + \int_{B_{4R_0'}(0)} \left(\left(u_k^2 \cdot \chi_{B_{8R_0'}(0)\setminus B_{4R_0'}(0)}\right) * Y_{a_k}\right) \\
&\qquad \leq -C_0 R_0'^3 + \frac{C_0}{4} R_0'^3 + \frac{C_0}{4} R_0'^3 = -\frac{C_0}{2} R_0'^3 \leq -1.
\end{aligned}
$$

Now choose $R = 4R_0' + 2$ such that $\psi = \psi_{R_0'} \in C_c^\infty(B_{R-2}(0))$ satisfies the estimate (A.18) for all $a_{\mathrm{c}} < a \leq a_0$. Then let $\xi \in C^\infty(\mathbb{R}^3)$ satisfy $0 \leq \xi \leq 1$, $\xi = 1$ on $B_{R-1}^c(0)$, $\xi = 0$ on $B_{R-2}(0)$ and for $\varepsilon > 0$, define $\varphi_{\varepsilon,k} \in H^1(\mathbb{R}^3)$ by

$$
\varphi_{\varepsilon,k}(x) = \varepsilon \psi(x) + \xi(x) u_k(x).
$$

It follows from the definition that $\varphi_{\varepsilon,k}$ satisfies the boundary condition from (A.9), that $\varphi_{\varepsilon,k}|_{\partial B_R(0)} = u_k$. Observe that as ψ and $\xi \cdot u_k$ have disjoint support, the energy $E(\varphi_{\varepsilon,k}; k, R)$ can be decomposed as

$$E(\varphi_{\varepsilon,k}; k, R) = E(\varepsilon\psi; k, R) + E(\xi u_k; k, R) \\ + \varepsilon^2 \int_{B_R(0)} \left((\xi u_k)^2 \cdot \chi_{B_R(0)} * Y_{a_k}\right) \psi^2.$$

Recall that ψ satisfies (A.18), so for $0 < \varepsilon \le 1$

$$\begin{aligned} E(\varepsilon\psi; k, R) + \varepsilon^4 = \varepsilon^2 &\left(\int_{B_R(0)} |\nabla\psi|^2 + \int_{B_R(0)} \left(\left(u_k^2 \cdot \chi_{B_R(0)^c} - m_k\right) * Y_{a_k}\right) \psi^2 \right) \\ &+ \varepsilon^{10/3} \int_{B_R(0)} \psi^{10/3} + \frac{\varepsilon^4}{2} \int_{B_R(0)} \left(\psi^2 \cdot \chi_{B_R(0)} * Y_{a_k}\right) \psi^2 + \varepsilon^4 \\ &\le -\varepsilon^2 + C\varepsilon^{10/3} R^3 + C\varepsilon^4 a_k^{-2} R^3 + \varepsilon^4 \\ &\le -\varepsilon^2 + C\varepsilon^4 =: -\varepsilon^2 + C_3\varepsilon^4. \end{aligned}$$

Choosing $\varepsilon = \varepsilon_0 = \min\{1, (2C_3)^{-1/2}\}$ implies that (A.22) holds

$$E(\varepsilon_0\psi; k, R) + \varepsilon_0^4 \le -\varepsilon_0^2 + C_3\varepsilon_0^4 \le -\frac{\varepsilon_0^2}{2} =: -C_1 < 0. \tag{A.22}$$

Now consider

$$\begin{aligned} E(\xi u_k; k, R) = &\int_{B_R(0)} |\nabla(\xi u_k)|^2 + \int_{B_R(0)} (\xi u_k)^{10/3} - \int_{B_R(0)} (m_k * Y_{a_k})\, (\xi u_k)^2 \\ &+ \frac{1}{2} \int_{B_R(0)} \left((\xi u_k)^2 \cdot \chi_{B_R(0)} * Y_{a_k}\right) (\xi u_k)^2 \\ &+ \int_{B_R(0)} \left(u_k^2 \cdot \chi_{B_R(0)^c} * Y_{a_k}\right) (\xi u_k)^2. \end{aligned}$$

Using that $0 \le \xi \le 1$, $|\nabla\xi| \in L^\infty(\mathbb{R}^3)$, $u_k \to 0$ as $k \to \infty$ and following the proof of (A.12), it follows that $E(\xi u_k; k, R) \to 0$ as $k \to \infty$. For the remaining term

$$\begin{aligned} 0 \le \varepsilon_0^2 \int_{B_R(0)} \left((\xi u_k)^2 \cdot \chi_{B_R(0)} * Y_{a_k}\right) \psi^2 &\le C\varepsilon_0^2 \|u_k\|_{L^\infty(B_R(0))}^2 \|Y_{a_k}\|_{L^1(\mathbb{R}^3)} \int_{B_R(0)} \psi^2 \\ &= \frac{C\varepsilon_0^2}{a_c^2} \|u_k\|_{L^\infty(B_R(0))}^2 \to 0 \text{ as } k \to \infty. \end{aligned}$$

It follows that there exists $k_2 \in \mathbb{N}$ such that for all $k \geq k_2$

$$E(\xi u_k; k, R) + \varepsilon_0^2 \int_{B_R(0)} \left((\xi u_k)^2 \cdot \chi_{B_R(0)} * Y_{a_k}\right) \psi^2 \leq \varepsilon_0^4. \tag{A.23}$$

Combining (A.22) and (A.23), for $k \geq \max\{k_1, k_2\}$ yields the desired estimate (A.17).

$$\begin{aligned} E(\varphi_{\varepsilon_0,k}; k, R) &= E(\varepsilon_0 \psi; k, R) + E(\xi u_k; k, R) \\ &\quad + \varepsilon_0^2 \int_{B_R(0)} \left((\xi u_k)^2 \cdot \chi_{B_R(0)} * Y_{a_k}\right) \psi^2 \\ &\leq E(\varepsilon_0 \psi; k, R) + \varepsilon_0^4 \leq -C_1 < 0, \end{aligned}$$

which contradicts the initial assumption (A.7), hence (A.6) and subsequently the desired estimate (A.1) hold. □

Proof of Proposition 2.15. The estimate (2.113) is shown by contradiction, so suppose there exists $a_0 > a_\mathrm{c}$ such that

$$\inf_{a_\mathrm{c} < a \leq a_0} \inf_{m \in \mathcal{M}_{L^2}(M,\omega)} \inf_{x \in \mathbb{R}^3} u_{a,m}(x) = 0,$$

hence for each $k \in \mathbb{N}$, there exists $a_k \in (a_\mathrm{c}, a_0], m_k \in \mathcal{M}_{L^2}(M, \omega)$ and $x_k \in \mathbb{R}^3$ such that $u_{a_k,m_k}(x_k) \leq \frac{1}{k}$. Without loss of generality, assume that $x_k = 0$ for all $k \in \mathbb{N}$, otherwise translate u_{a_k,m_k}. For convenience, u_{a_k,m_k} will be referred to as u_k in this argument. Applying the argument used to show (A.8) verbatim, the Harnack inequality implies that u_k converges uniformly to 0 on compact sets.

For $R > 0$ and $k \in \mathbb{N}$, define the energy functional acting on v satisfying $\nabla v \in L^2(B_R(0))$ and $v \in L^{10/3}(B_R(0))$ by

$$\begin{aligned} E(v; k, R) = &\int_{B_R(0)} |\nabla v|^2 + \int_{B_R(0)} v^{10/3} - \int_{B_R(0)} (m_k * Y_{a_k})\, v^2 \\ &+ \frac{1}{2} \int_{B_R(0)} \left(v^2 \cdot \chi_{B_R(0)} * Y_{a_k}\right) v^2 + \int_{B_R(0)} \left(u_k^2 \cdot \chi_{B_R(0)^\mathrm{c}} * Y_{a_k}\right) v^2. \end{aligned} \tag{A.24}$$

Then consider the corresponding variational problem

$$I(k,R) = \inf\left\{E(v;k,R)\,\middle|\, \nabla v \in L^2(B_R(0)), v \in L^{10/3}(B_R(0)), v|_{\partial B_R(0)} = u_k\right\}. \tag{A.25}$$

The construction of the energy (A.24) and the boundary condition of (A.25) ensures that u_k is the unique minimiser of (A.25) for each $R > 0$. It follows that for any fixed $R > 0$, $I(k,R) \to 0$ as $k \to \infty$. Then by following the construction used in the proof of Lemma A.1, there exists $R > 0$ and $\varphi_{\varepsilon,k}$ such that for sufficiently small $\varepsilon > 0$ and sufficiently large $k \in \mathbb{N}$

$$I(k,R) = E(u_k;k,R) \le E(\varphi_{\varepsilon,k};k,R) \le -C_1 < 0,$$

which contradicts the fact that $I(k,R) \to 0$ as $k \to \infty$, hence the desired estimate (2.113) holds.

Consequently, as for all $a > 0$ and $m \in \mathcal{M}_{L^2}(M,\omega)$, the electron density satisfies $\inf u_a > 0$, the argument presented in [16, Chapter 6] can be applied verbatim to guarantee the uniqueness of the corresponding ground state (u_a, ϕ_a). □

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